



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:04 PM UTC

PDB ID : 7PI3 / pdb_00007pi3
Title : PfCyRPA bound to Fab fragments from monoclonal antibodies Cy.003, Cy.004 and Cy.007
Authors : Ragotte, R.J.; Higgins, M.K.
Deposited on : 2021-08-19
Resolution : 3.27 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

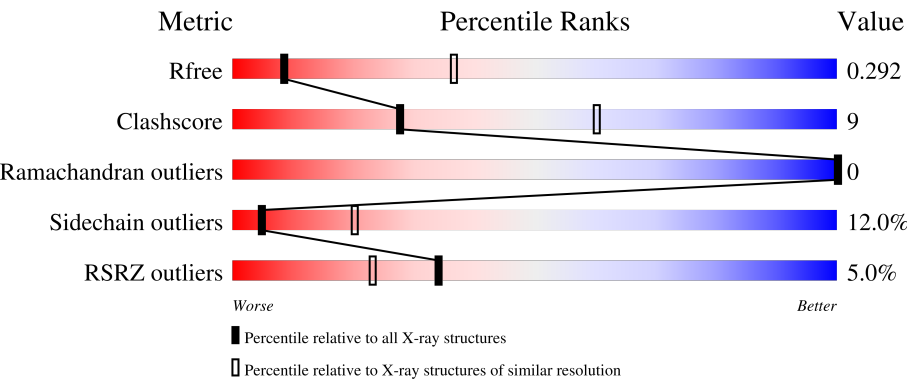
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	343	4% 52% 36% 6%
1	H	343	6% 59% 30% 5% 6%
1	O	343	2% 59% 31% 6% 5%
1	V	343	4% 57% 32% 5% 5%
2	B	230	4% 69% 25%

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Mol	Chain	Length	Quality of chain
2	I	230	
2	P	230	
2	W	230	
3	C	210	
3	J	210	
3	Q	210	
3	X	210	
4	D	230	
4	K	230	
4	R	230	
4	Y	230	
5	E	209	
5	L	209	
5	S	209	
5	Z	209	
6	F	321	
6	M	321	
6	T	321	
6	a	321	
7	G	209	
7	N	209	
7	U	209	
7	b	209	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 48847 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cysteine-rich protective antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2730	1755	439	523	13			
1	H	321	Total	C	N	O	S	0	0	0
			2675	1723	429	510	13			
1	O	327	Total	C	N	O	S	0	0	0
			2722	1751	438	520	13			
1	V	325	Total	C	N	O	S	0	0	0
			2705	1741	435	516	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ALA	SER	conflict	UNP Q8IFM8
A	324	ALA	THR	conflict	UNP Q8IFM8
A	340	ALA	THR	conflict	UNP Q8IFM8
A	363	GLY	-	expression tag	UNP Q8IFM8
A	364	GLY	-	expression tag	UNP Q8IFM8
A	365	GLY	-	expression tag	UNP Q8IFM8
A	366	GLY	-	expression tag	UNP Q8IFM8
A	367	SER	-	expression tag	UNP Q8IFM8
A	368	GLU	-	expression tag	UNP Q8IFM8
A	369	PRO	-	expression tag	UNP Q8IFM8
A	370	GLU	-	expression tag	UNP Q8IFM8
A	371	ALA	-	expression tag	UNP Q8IFM8
H	147	ALA	SER	conflict	UNP Q8IFM8
H	324	ALA	THR	conflict	UNP Q8IFM8
H	340	ALA	THR	conflict	UNP Q8IFM8
H	363	GLY	-	expression tag	UNP Q8IFM8
H	364	GLY	-	expression tag	UNP Q8IFM8
H	365	GLY	-	expression tag	UNP Q8IFM8
H	366	GLY	-	expression tag	UNP Q8IFM8
H	367	SER	-	expression tag	UNP Q8IFM8
H	368	GLU	-	expression tag	UNP Q8IFM8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	369	PRO	-	expression tag	UNP Q8IFM8
H	370	GLU	-	expression tag	UNP Q8IFM8
H	371	ALA	-	expression tag	UNP Q8IFM8
O	147	ALA	SER	conflict	UNP Q8IFM8
O	324	ALA	THR	conflict	UNP Q8IFM8
O	340	ALA	THR	conflict	UNP Q8IFM8
O	363	GLY	-	expression tag	UNP Q8IFM8
O	364	GLY	-	expression tag	UNP Q8IFM8
O	365	GLY	-	expression tag	UNP Q8IFM8
O	366	GLY	-	expression tag	UNP Q8IFM8
O	367	SER	-	expression tag	UNP Q8IFM8
O	368	GLU	-	expression tag	UNP Q8IFM8
O	369	PRO	-	expression tag	UNP Q8IFM8
O	370	GLU	-	expression tag	UNP Q8IFM8
O	371	ALA	-	expression tag	UNP Q8IFM8
V	147	ALA	SER	conflict	UNP Q8IFM8
V	324	ALA	THR	conflict	UNP Q8IFM8
V	340	ALA	THR	conflict	UNP Q8IFM8
V	363	GLY	-	expression tag	UNP Q8IFM8
V	364	GLY	-	expression tag	UNP Q8IFM8
V	365	GLY	-	expression tag	UNP Q8IFM8
V	366	GLY	-	expression tag	UNP Q8IFM8
V	367	SER	-	expression tag	UNP Q8IFM8
V	368	GLU	-	expression tag	UNP Q8IFM8
V	369	PRO	-	expression tag	UNP Q8IFM8
V	370	GLU	-	expression tag	UNP Q8IFM8
V	371	ALA	-	expression tag	UNP Q8IFM8

- Molecule 2 is a protein called Monoclonal antibody Cy.003 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	0	0	0
			1611	1009	276	319	7			
2	I	221	Total	C	N	O	S	132	0	0
			1611	1009	276	319	7			
2	P	221	Total	C	N	O	S	442	0	0
			1611	1009	276	319	7			
2	W	218	Total	C	N	O	S	0	0	0
			1597	1002	273	315	7			

- Molecule 3 is a protein called Monoclonal antibody Cy.003 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	0
			1552	963	263	322	4			
3	J	207	Total	C	N	O	S	102	0	0
			1552	963	263	322	4			
3	Q	207	Total	C	N	O	S	580	0	0
			1552	963	263	322	4			
3	X	206	Total	C	N	O	S	0	0	0
			1547	960	262	321	4			

- Molecule 4 is a protein called Monoclonal antibody Cy.007 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	221	Total	C	N	O	S	621	0	0
			1619	1013	272	327	7			
4	K	220	Total	C	N	O	S	690	0	0
			1614	1010	271	326	7			
4	R	221	Total	C	N	O	S	690	0	0
			1619	1013	272	327	7			
4	Y	221	Total	C	N	O	S	621	0	0
			1619	1013	272	327	7			

- Molecule 5 is a protein called Monoclonal antibody Cy.007 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	204	Total	C	N	O	S	777	0	0
			1541	957	262	318	4			
5	L	203	Total	C	N	O	S	777	0	0
			1536	954	261	317	4			
5	S	200	Total	C	N	O	S	796	0	0
			1517	942	258	313	4			
5	Z	203	Total	C	N	O	S	777	0	0
			1537	955	261	317	4			

- Molecule 6 is a protein called Monoclonal antibody Cy.004 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	223	Total	C	N	O	S	685	0	0
			1634	1023	277	329	5			
6	M	223	Total	C	N	O	S	493	0	0
			1634	1023	277	329	5			
6	T	218	Total	C	N	O	S	533	0	0
			1603	1005	271	322	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	a	219	Total	C	N	O	S	660	0	0
			1604	1004	272	323	5			

- Molecule 7 is a protein called Monoclonal antibody Cy.004 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	209	Total	C	N	O	S	834	0	0
			1577	978	265	329	5			
7	N	209	Total	C	N	O	S	30	0	0
			1577	978	265	329	5			
7	U	208	Total	C	N	O	S	359	0	0
			1572	975	264	328	5			
7	b	208	Total	C	N	O	S	535	0	0
			1571	975	264	328	4			

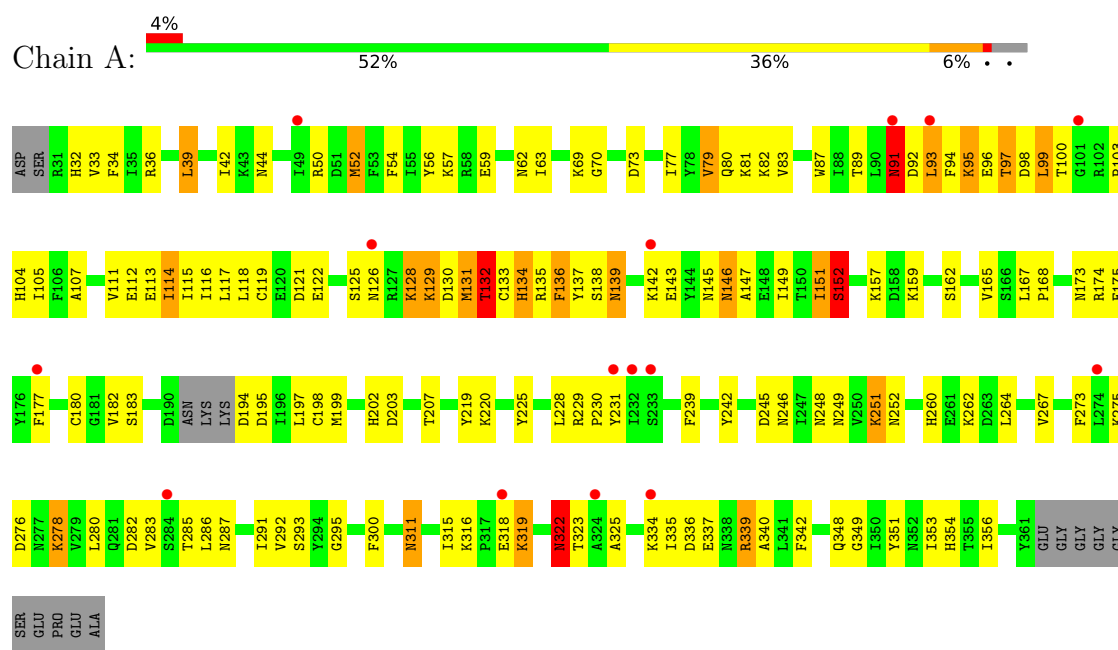
- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	2	Total	Ca	2	0
			2	2		
8	H	1	Total	Ca	1	0
			1	1		
8	M	1	Total	Ca	1	0
			1	1		
8	T	2	Total	Ca	2	0
			2	2		
8	a	2	Total	Ca	2	0
			2	2		

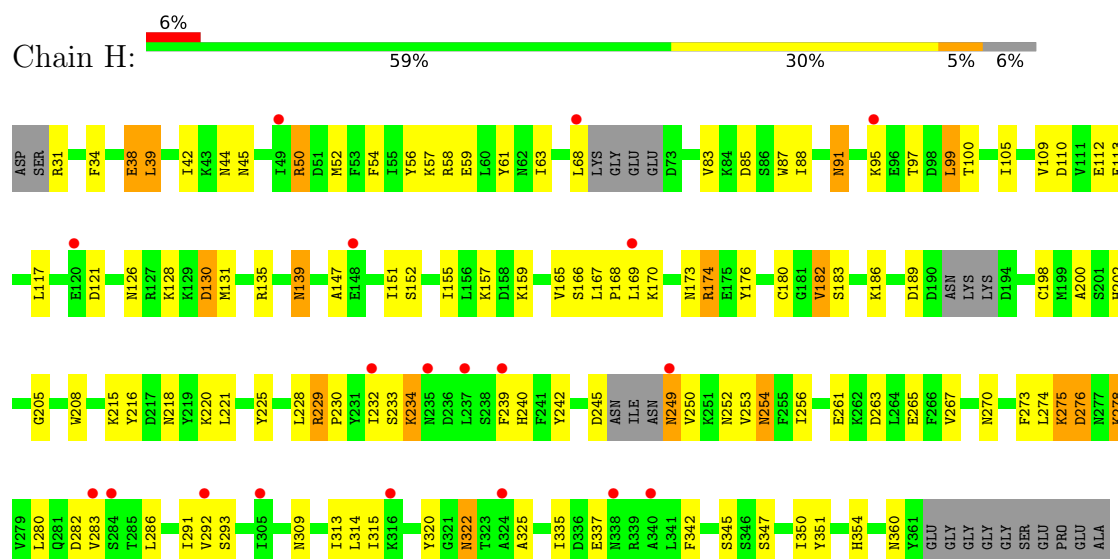
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cysteine-rich protective antigen



• Molecule 1: Cysteine-rich protective antigen



Chain O:

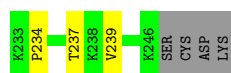
Chain V:

4% 57% 32% 5% 5%

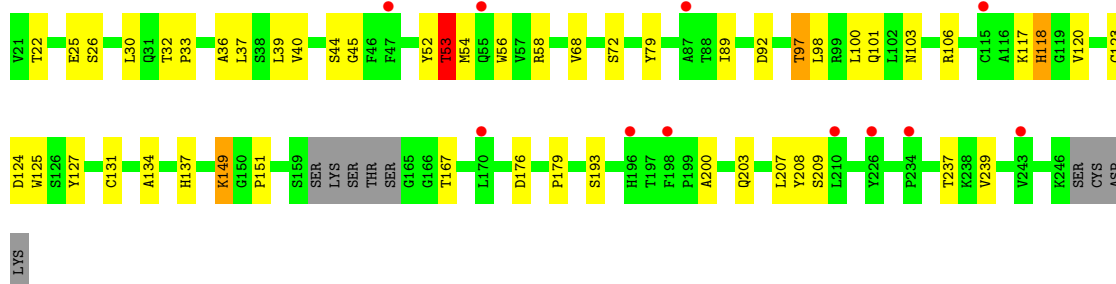
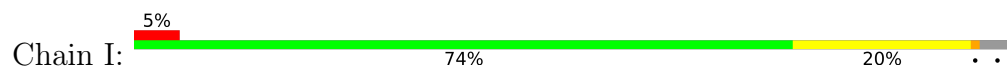
Chain B:

4% 69% 25%

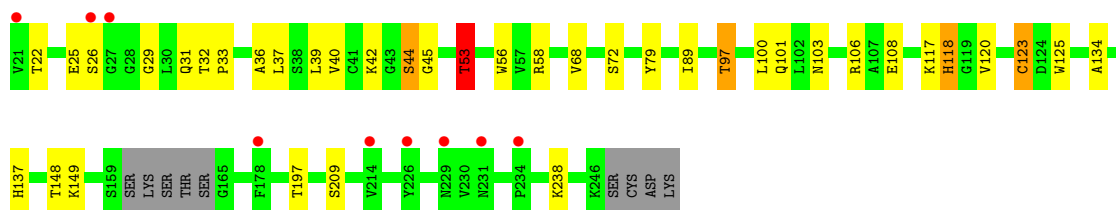
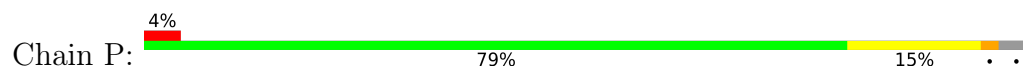
W21 T22 L23 D24 E25 L30 L37 S38 V40 C41 G42 G43 S44 F49 S50 S51 Y52 T53 M54 Q55 W56 Y79 G80 A81 K84 A87 T88 I89 S90 L98 R99 L102 R106 A107 E108 D109 T110 G111 T112 Y113 V114 C115 A116 K117 H118 V120 C123 F124 W125 S126 Y127 A134 W135 G136 H137 I142 S145 K149 G150 P151 S152 A157 P158 S159 SER LYS LYS THR SER L170 K175 D176 Y177 F178 P179 E180 S185 W186 L191 H196 T197 F198 S204 L207 S211 S212 V213 V214 I227 C228 N229 W230



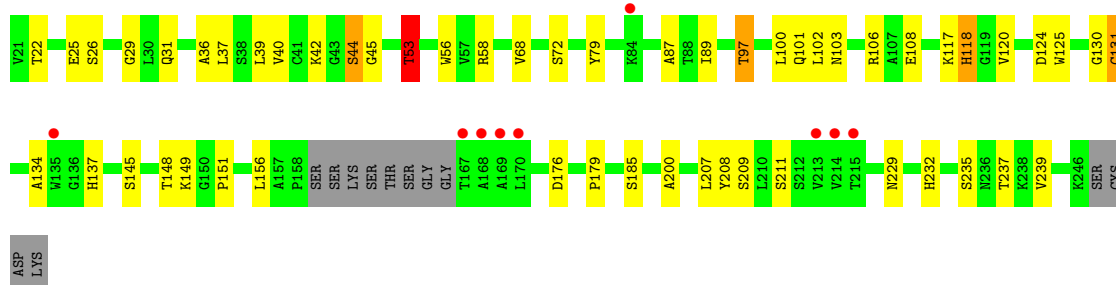
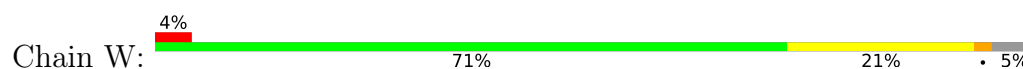
• Molecule 2: Monoclonal antibody Cy.003 heavy chain



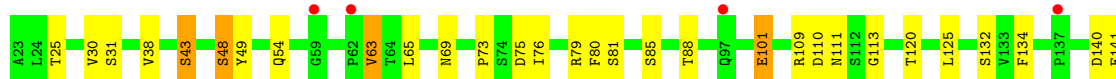
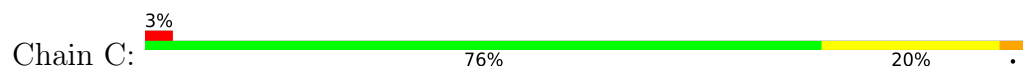
• Molecule 2: Monoclonal antibody Cy.003 heavy chain



• Molecule 2: Monoclonal antibody Cy.003 heavy chain

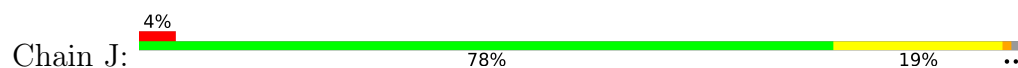


• Molecule 3: Monoclonal antibody Cy.003 light chain

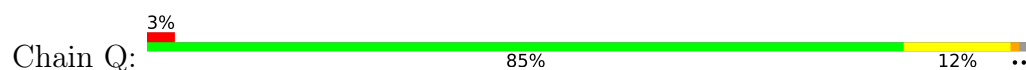




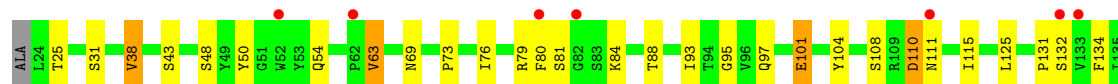
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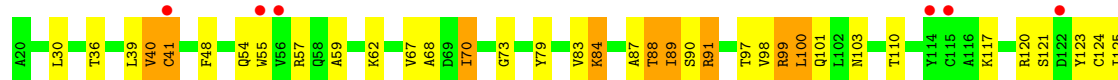
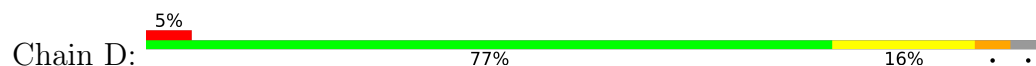
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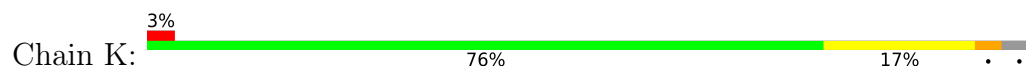
• Molecule 3: Monoclonal antibody Cy.003 light chain

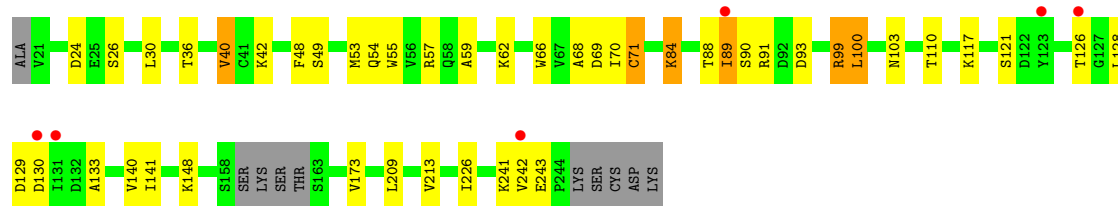


• Molecule 4: Monoclonal antibody Cy.007 heavy chain

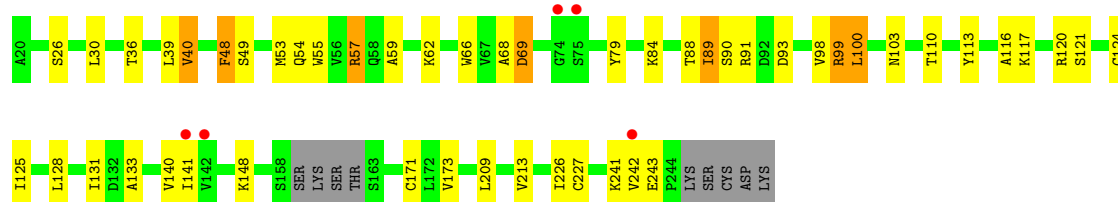
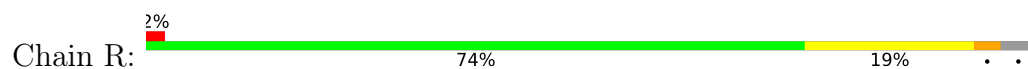


• Molecule 4: Monoclonal antibody Cy.007 heavy chain

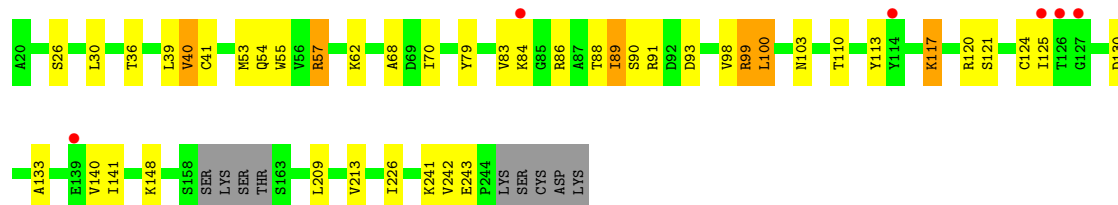
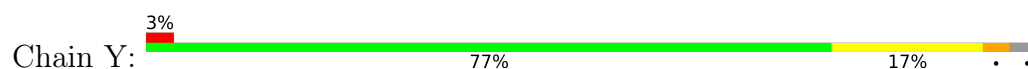




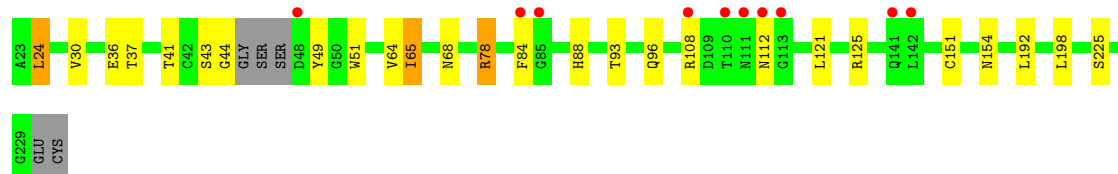
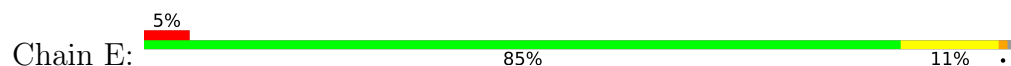
• Molecule 4: Monoclonal antibody Cy.007 heavy chain



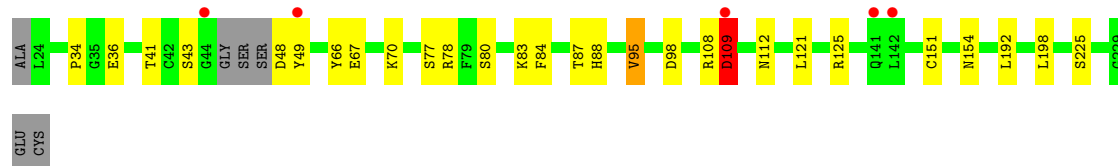
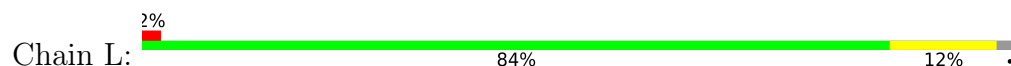
• Molecule 4: Monoclonal antibody Cy.007 heavy chain



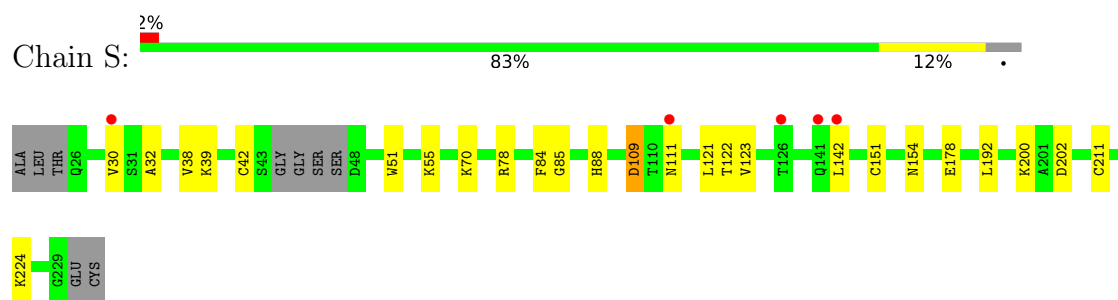
• Molecule 5: Monoclonal antibody Cy.007 light chain



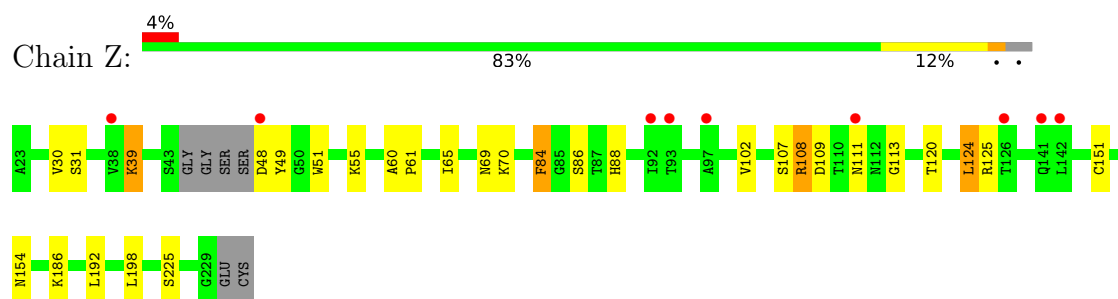
• Molecule 5: Monoclonal antibody Cy.007 light chain



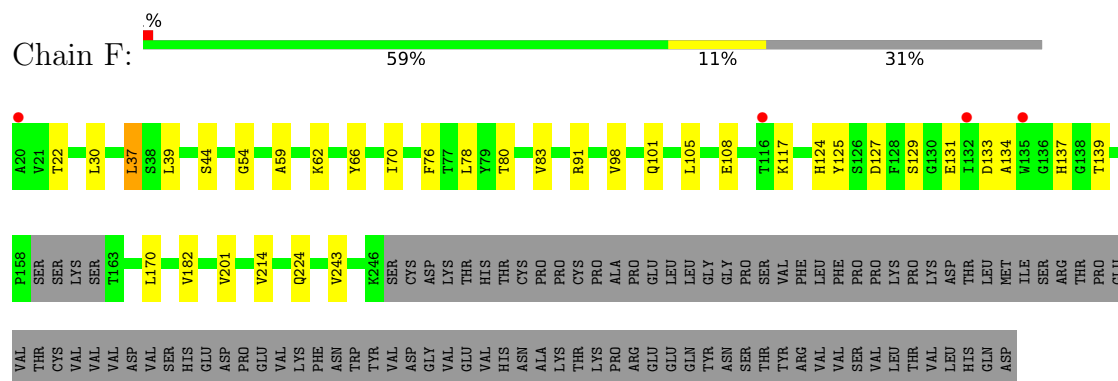
• Molecule 5: Monoclonal antibody Cy.007 light chain



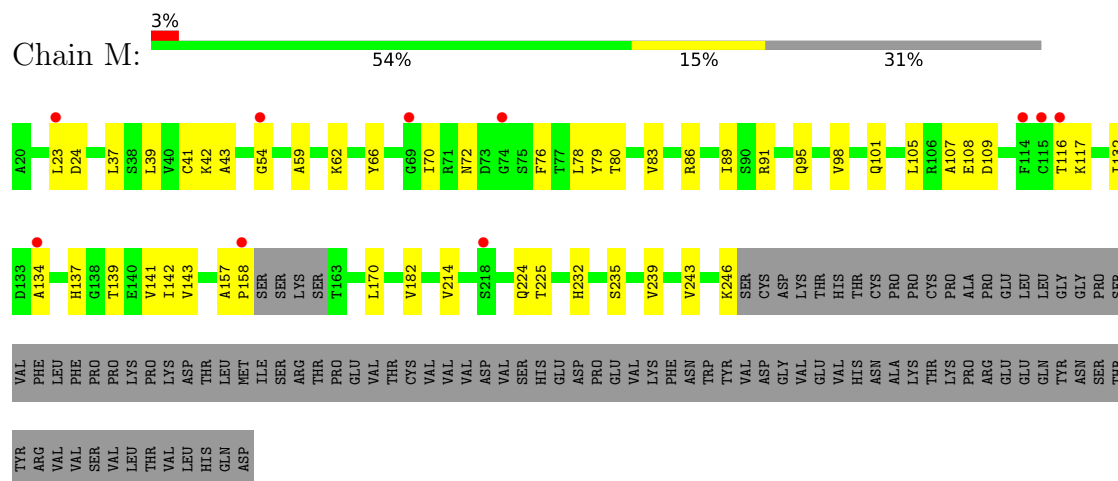
- Molecule 5: Monoclonal antibody Cy.007 light chain



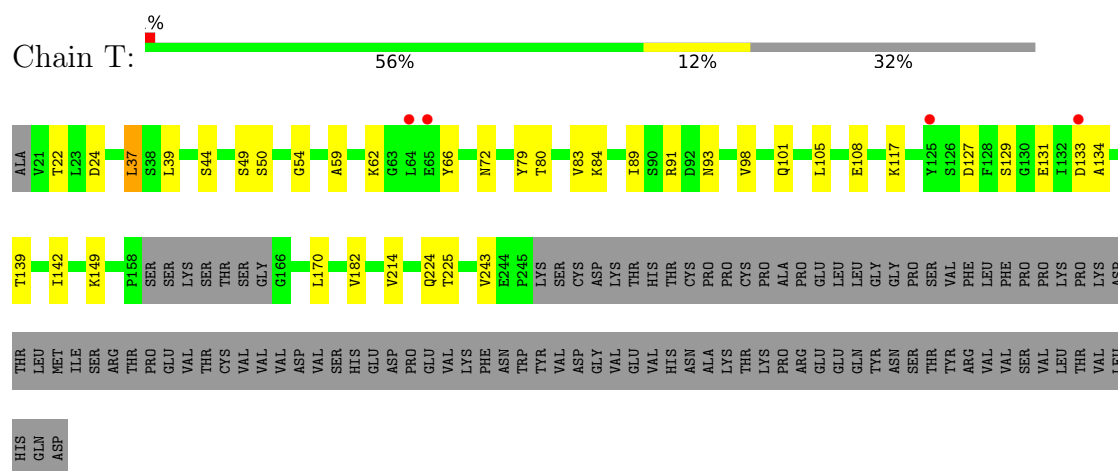
- Molecule 6: Monoclonal antibody Cy.004 heavy chain



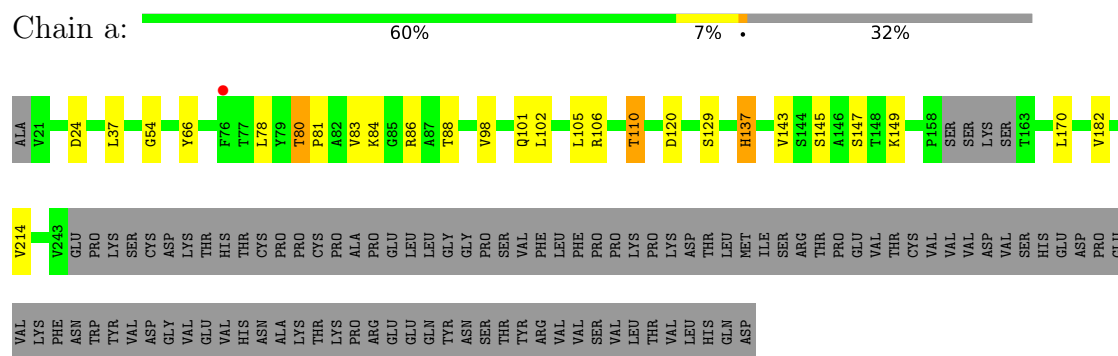
- Molecule 6: Monoclonal antibody Cy.004 heavy chain



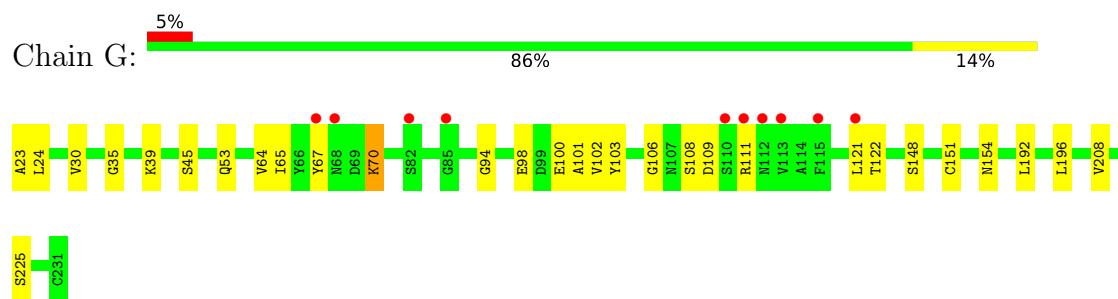
- Molecule 6: Monoclonal antibody Cy.004 heavy chain



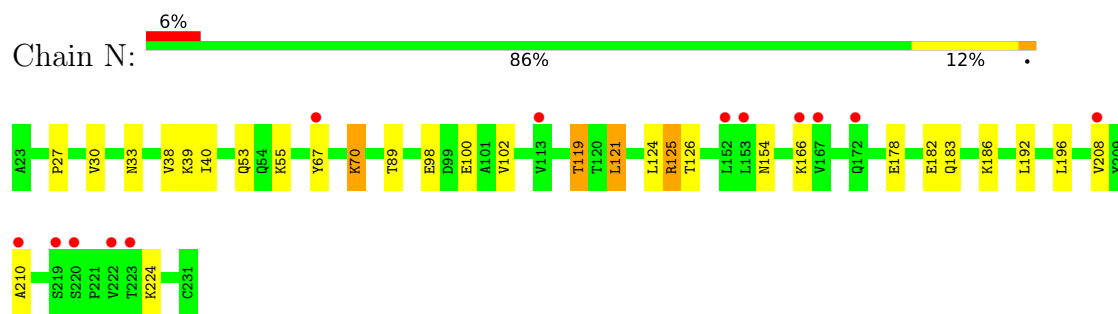
- Molecule 6: Monoclonal antibody Cy.004 heavy chain



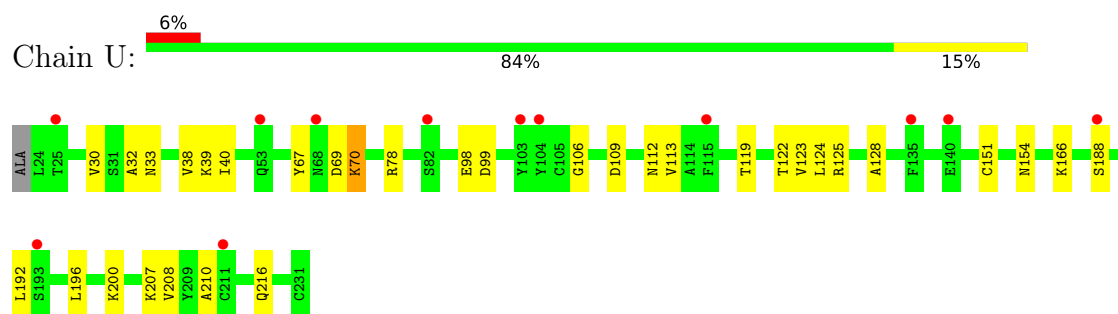
- Molecule 7: Monoclonal antibody Cy.004 light chain



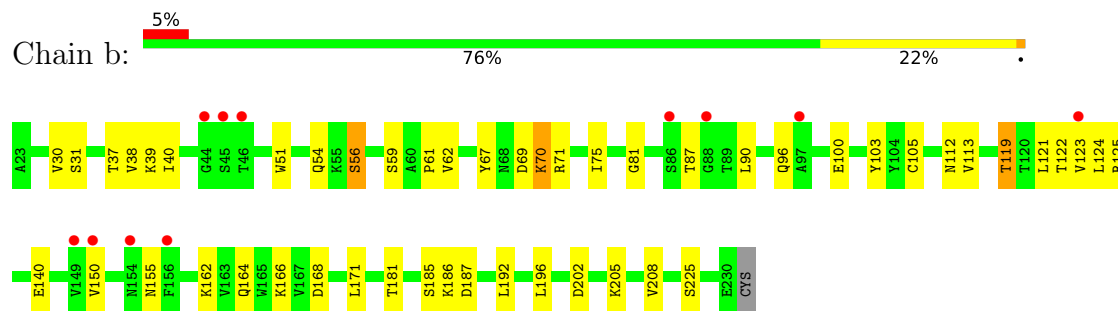
- Molecule 7: Monoclonal antibody Cy.004 light chain



- Molecule 7: Monoclonal antibody Cy.004 light chain



- Molecule 7: Monoclonal antibody Cy.004 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	164.84Å 164.84Å 382.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.64 – 3.27 47.64 – 3.27	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.64-3.27) 99.9 (47.64-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.10.4 (20-OCT-2021)	Depositor
R, R_{free}	0.285 , 0.298 0.280 , 0.292	Depositor DCC
R_{free} test set	7806 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	113.8	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 121.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.107 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	48847	wwPDB-VP
Average B, all atoms (Å ²)	187.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.92	8/2793 (0.3%)	1.21	11/3772 (0.3%)
1	H	0.67	1/2736 (0.0%)	1.06	5/3693 (0.1%)
1	O	0.68	1/2785 (0.0%)	1.07	6/3761 (0.2%)
1	V	0.67	0/2768	1.04	5/3739 (0.1%)
2	B	0.65	1/1648 (0.1%)	1.15	7/2243 (0.3%)
2	I	0.61	0/1648	1.02	3/2243 (0.1%)
2	P	0.58	0/1648	1.00	4/2243 (0.2%)
2	W	0.63	0/1634	1.02	3/2225 (0.1%)
3	C	0.63	0/1584	0.98	1/2153 (0.0%)
3	J	0.61	0/1584	0.98	0/2153
3	Q	0.59	0/1584	0.97	0/2153
3	X	0.62	0/1579	1.01	4/2146 (0.2%)
4	D	0.55	0/1654	0.91	1/2254 (0.0%)
4	K	0.56	0/1649	0.94	6/2247 (0.3%)
4	R	0.56	0/1654	0.94	4/2254 (0.2%)
4	Y	0.55	0/1654	0.92	0/2254
5	E	0.57	0/1573	0.90	1/2139 (0.0%)
5	L	0.57	0/1568	0.92	1/2132 (0.0%)
5	S	0.57	0/1549	0.91	2/2106 (0.1%)
5	Z	0.57	0/1569	0.91	0/2134
6	F	0.56	0/1670	0.92	1/2273 (0.0%)
6	M	0.58	0/1670	0.96	1/2273 (0.0%)
6	T	0.56	0/1639	0.91	1/2232 (0.0%)
6	a	0.59	0/1639	0.95	0/2231
7	G	0.56	0/1610	0.93	1/2192 (0.0%)
7	N	0.59	0/1610	0.96	0/2192
7	U	0.58	0/1605	0.95	1/2185 (0.0%)
7	b	0.61	0/1604	0.97	1/2184 (0.0%)
All	All	0.63	11/49908 (0.0%)	0.99	70/67806 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	PHE	CA-C	9.24	1.63	1.52
1	A	131	MET	SD-CE	-8.58	1.58	1.79
2	B	180	GLU	CA-C	6.69	1.60	1.52
1	A	138	SER	CA-C	6.36	1.60	1.52
1	A	132	THR	CA-C	-5.95	1.46	1.53
1	O	124	PHE	CA-C	5.88	1.58	1.52
1	A	152	SER	C-N	5.49	1.41	1.33
1	A	91	ASN	CA-C	5.42	1.60	1.52
1	A	112	GLU	CA-C	-5.42	1.45	1.52
1	H	83	VAL	CA-C	5.06	1.59	1.52
1	A	113	GLU	CA-C	-5.00	1.46	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ASN	CA-CB-CG	10.55	123.15	112.60
5	L	109	ASP	CA-CB-CG	7.88	120.48	112.60
2	B	179	PRO	CA-C-N	7.22	128.65	120.06
2	B	179	PRO	C-N-CA	7.22	128.65	120.06
2	B	204	SER	CA-C-N	6.98	129.96	120.54
2	B	204	SER	C-N-CA	6.98	129.96	120.54
3	X	95	GLY	CA-C-N	6.69	130.46	120.69
3	X	95	GLY	C-N-CA	6.69	130.46	120.69
1	O	91	ASN	CA-CB-CG	6.62	119.22	112.60
1	A	34	PHE	CA-CB-CG	6.61	120.41	113.80
1	O	189	ASP	CA-CB-CG	6.46	119.06	112.60
4	D	48	PHE	CA-CB-CG	6.44	120.24	113.80
1	V	91	ASN	CA-CB-CG	6.43	119.03	112.60
1	H	91	ASN	CA-CB-CG	6.40	119.00	112.60
1	O	276	ASP	CA-CB-CG	6.23	118.83	112.60
4	R	48	PHE	CA-CB-CG	6.17	119.97	113.80
1	H	276	ASP	CA-CB-CG	6.07	118.67	112.60
2	B	55	GLN	N-CA-C	6.07	118.40	109.24
1	A	138	SER	N-CA-C	6.01	119.28	109.06
1	O	34	PHE	CA-CB-CG	5.94	119.74	113.80
1	H	34	PHE	CA-CB-CG	5.92	119.72	113.80
7	b	100	GLU	CB-CG-CD	5.90	122.63	112.60
2	I	53	THR	CB-CA-C	5.88	119.71	110.19
1	H	85	ASP	N-CA-C	-5.85	103.53	111.55
2	P	53	THR	CB-CA-C	5.83	119.63	110.19
2	P	79	TYR	CA-C-N	5.81	125.61	120.10
2	P	79	TYR	C-N-CA	5.81	125.61	120.10
5	S	111	ASN	CA-CB-CG	5.79	118.39	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	69	ASP	CA-CB-CG	5.77	118.37	112.60
1	V	336	ASP	CA-CB-CG	5.77	118.37	112.60
2	W	53	THR	CB-CA-C	5.77	119.53	110.19
3	X	205	GLU	CA-C-N	5.76	128.31	120.54
3	X	205	GLU	C-N-CA	5.76	128.31	120.54
2	B	175	LYS	CA-C-O	-5.71	114.43	120.71
2	I	79	TYR	CA-C-N	5.70	125.51	120.10
2	I	79	TYR	C-N-CA	5.70	125.51	120.10
1	V	34	PHE	CA-CB-CG	5.68	119.48	113.80
2	W	79	TYR	CA-C-N	5.66	125.47	120.10
2	W	79	TYR	C-N-CA	5.66	125.47	120.10
5	S	109	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	142	LYS	O-C-N	5.59	128.19	121.76
7	U	69	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	137	TYR	N-CA-C	5.52	117.89	108.90
1	O	336	ASP	CA-CB-CG	5.50	118.10	112.60
4	K	69	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	92	ASP	N-CA-C	-5.46	98.87	108.20
1	A	276	ASP	CA-CB-CG	5.44	118.04	112.60
1	V	245	ASP	CA-CB-CG	5.41	118.01	112.60
7	G	102	VAL	N-CA-CB	5.34	117.09	111.00
1	A	79	VAL	N-CA-C	-5.27	101.93	108.89
6	T	133	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	92	ASP	CA-CB-CG	5.26	117.86	112.60
1	V	226	PHE	CA-CB-CG	5.23	119.03	113.80
4	R	49	SER	CA-C-N	5.19	129.69	121.44
4	R	49	SER	C-N-CA	5.19	129.69	121.44
1	O	245	ASP	CA-CB-CG	5.19	117.79	112.60
2	P	123	CYS	N-CA-C	5.15	115.33	108.38
6	F	133	ASP	CA-CB-CG	5.14	117.74	112.60
3	C	75	ASP	CA-CB-CG	5.11	117.70	112.60
5	E	65	ILE	CB-CA-C	5.11	117.06	110.12
4	K	49	SER	CA-C-N	5.09	129.53	121.44
4	K	49	SER	C-N-CA	5.09	129.53	121.44
6	M	141	VAL	N-CA-CB	5.06	118.58	112.10
1	H	189	ASP	CA-CB-CG	5.04	117.64	112.60
4	K	48	PHE	CA-CB-CG	5.04	118.84	113.80
1	A	322	ASN	CA-C-N	5.03	127.28	120.44
1	A	322	ASN	C-N-CA	5.03	127.28	120.44
2	B	227	ILE	N-CA-C	5.02	115.08	107.80
4	K	71	CYS	CA-C-N	5.01	128.00	120.69
4	K	71	CYS	C-N-CA	5.01	128.00	120.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2730	0	2615	103	0
1	H	2675	0	2562	69	0
1	O	2722	0	2611	72	0
1	V	2705	0	2594	76	0
2	B	1611	0	1561	45	0
2	I	1611	0	1561	29	0
2	P	1611	0	1561	21	0
2	W	1597	0	1550	30	0
3	C	1552	0	1499	26	0
3	J	1552	0	1499	21	0
3	Q	1552	0	1499	6	0
3	X	1547	0	1494	23	0
4	D	1619	0	1570	20	0
4	K	1614	0	1565	20	0
4	R	1619	0	1570	18	0
4	Y	1619	0	1570	14	0
5	E	1541	0	1479	7	0
5	L	1536	0	1474	8	0
5	S	1517	0	1453	6	0
5	Z	1537	0	1476	10	0
6	F	1634	0	1582	14	0
6	M	1634	0	1582	16	0
6	T	1603	0	1549	15	0
6	a	1604	0	1551	8	0
7	G	1577	0	1513	11	0
7	N	1577	0	1513	9	0
7	U	1572	0	1508	12	0
7	b	1571	0	1508	10	0
8	F	2	0	0	0	0
8	H	1	0	0	0	0
8	M	1	0	0	0	0
8	T	2	0	0	0	0
8	a	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	48847	0	47069	661	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (661) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:130:ASP:HB3	1:V:152:SER:HA	1.19	1.15
7:U:40:ILE:HG21	7:U:119:THR:HG21	1.47	0.95
1:V:68:LEU:HB2	1:V:73:ASP:HB3	1.49	0.91
1:A:130:ASP:HB3	1:A:152:SER:HA	1.53	0.91
1:A:130:ASP:CB	1:A:152:SER:HA	2.05	0.86
4:D:88:THR:HG23	4:D:101:GLN:HB2	1.55	0.85
4:Y:55:TRP:HE1	4:Y:98:VAL:HG12	1.44	0.82
4:K:55:TRP:CD1	4:K:100:LEU:HD23	2.14	0.81
1:A:79:VAL:HG23	1:A:93:LEU:HD11	1.63	0.80
1:A:131:MET:HB3	1:A:151:ILE:HG13	1.63	0.79
4:Y:55:TRP:HE1	4:Y:98:VAL:CG1	1.96	0.77
1:H:39:LEU:HG	1:H:354:HIS:CE1	2.20	0.77
1:V:39:LEU:HG	1:V:354:HIS:CE1	2.19	0.77
1:O:39:LEU:HG	1:O:354:HIS:CE1	2.19	0.76
3:C:79:ARG:NH1	3:C:80:PHE:HE1	1.85	0.75
2:B:56:TRP:HD1	2:B:89:ILE:HD12	1.51	0.75
3:C:79:ARG:HH11	3:C:80:PHE:HE1	1.32	0.75
2:B:185:SER:O	2:B:229:ASN:HB2	1.87	0.74
2:I:92:ASP:HB3	2:I:97:THR:HG23	1.69	0.74
1:A:315:ILE:HB	1:A:354:HIS:HE1	1.52	0.74
1:H:174:ARG:NH1	1:H:202:HIS:HD2	1.86	0.74
3:J:79:ARG:NH1	3:J:80:PHE:HE1	1.87	0.73
1:O:174:ARG:NH1	1:O:202:HIS:HD2	1.86	0.72
1:A:315:ILE:HB	1:A:354:HIS:CE1	2.24	0.72
1:O:151:ILE:CD1	1:O:208:TRP:HD1	2.04	0.71
3:J:79:ARG:HH11	3:J:80:PHE:HE1	1.38	0.71
1:V:130:ASP:CB	1:V:152:SER:HA	2.10	0.71
1:V:174:ARG:NH1	1:V:202:HIS:HD2	1.88	0.71
1:A:39:LEU:HD21	1:A:354:HIS:CD2	2.26	0.70
1:V:37:THR:HG21	1:V:313:ILE:HD13	1.72	0.70
1:V:283:VAL:HG22	1:V:292:VAL:HG12	1.72	0.70
1:H:151:ILE:CD1	1:H:208:TRP:HD1	2.04	0.70
2:W:185:SER:HB2	2:W:229:ASN:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:283:VAL:HG22	1:O:292:VAL:HG12	1.74	0.69
1:O:286:LEU:HB2	1:O:291:ILE:HD11	1.74	0.69
1:V:151:ILE:CD1	1:V:208:TRP:HD1	2.05	0.69
6:M:117:LYS:HB3	6:M:134:ALA:HB3	1.75	0.69
1:A:342:PHE:HB3	1:A:354:HIS:HB2	1.75	0.69
6:T:117:LYS:HB3	6:T:134:ALA:HB3	1.74	0.69
1:A:122:GLU:HA	1:A:126:ASN:HB2	1.74	0.68
1:V:286:LEU:HB2	1:V:291:ILE:HD11	1.75	0.68
1:H:283:VAL:HG22	1:H:292:VAL:HG12	1.75	0.67
1:A:80:GLN:HG2	1:A:89:THR:HA	1.76	0.67
1:A:322:ASN:HB3	1:A:325:ALA:HB2	1.77	0.67
3:C:31:SER:HB3	3:C:125:LEU:HD21	1.76	0.67
1:H:286:LEU:HB2	1:H:291:ILE:HD11	1.77	0.67
3:C:101:GLU:HG3	3:C:184:GLN:HB3	1.76	0.67
4:R:57:ARG:NH1	4:R:113:TYR:OH	2.27	0.67
1:A:39:LEU:HD21	1:A:354:HIS:NE2	2.10	0.67
1:H:240:HIS:HE2	1:H:253:VAL:HG11	1.59	0.66
1:A:117:LEU:HD21	1:A:149:ILE:HD11	1.77	0.66
1:V:240:HIS:HE2	1:V:253:VAL:HG11	1.60	0.66
3:Q:31:SER:HB3	3:Q:125:LEU:HD21	1.78	0.66
3:X:31:SER:HB3	3:X:125:LEU:HD21	1.78	0.66
4:D:68:ALA:HB1	4:D:89:ILE:HD13	1.76	0.66
5:Z:51:TRP:HE1	5:Z:88:HIS:CE1	2.13	0.66
2:I:25:GLU:O	2:I:137:HIS:HE1	1.78	0.66
3:J:101:GLU:HG3	3:J:184:GLN:HB3	1.77	0.66
3:X:101:GLU:HG3	3:X:184:GLN:HB3	1.78	0.66
1:V:322:ASN:HB3	1:V:325:ALA:HB2	1.78	0.66
1:A:93:LEU:O	1:A:96:GLU:HG2	1.97	0.65
1:H:322:ASN:HB3	1:H:325:ALA:HB2	1.77	0.65
3:J:31:SER:HB3	3:J:125:LEU:HD21	1.78	0.65
1:A:286:LEU:HD12	1:A:291:ILE:HG12	1.78	0.65
1:O:240:HIS:HE2	1:O:253:VAL:HG11	1.61	0.65
2:P:25:GLU:O	2:P:137:HIS:HE1	1.79	0.65
3:X:167:LYS:HG3	3:X:170:ASN:HA	1.77	0.65
4:Y:57:ARG:NH1	4:Y:113:TYR:OH	2.29	0.65
6:a:37:LEU:HD23	6:a:105:LEU:HD21	1.79	0.65
1:V:314:LEU:HG	1:V:316:LYS:HZ1	1.61	0.65
5:E:51:TRP:HE1	5:E:88:HIS:CE1	2.15	0.64
4:K:130:ASP:HA	5:L:66:TYR:HB2	1.79	0.64
3:X:132:SER:HB2	3:X:155:ASN:HB3	1.78	0.64
2:B:40:VAL:HG22	2:B:99:ARG:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:HIS:HE1	3:C:156:ASN:HD21	1.43	0.64
1:O:151:ILE:HD11	1:O:208:TRP:HD1	1.61	0.64
1:A:203:ASP:OD2	1:A:207:THR:HG23	1.98	0.64
4:Y:68:ALA:HB1	4:Y:89:ILE:HD13	1.78	0.64
3:X:79:ARG:NH1	3:X:80:PHE:HE2	1.95	0.64
4:R:68:ALA:HB1	4:R:89:ILE:HD13	1.78	0.64
6:F:117:LYS:HB3	6:F:134:ALA:HB3	1.80	0.63
1:H:170:LYS:NZ	1:H:173:ASN:H	1.95	0.63
1:O:54:PHE:HB3	1:O:165:VAL:HG11	1.80	0.63
1:A:42:ILE:HD12	1:A:353:ILE:HD11	1.80	0.63
1:H:151:ILE:HD11	1:H:208:TRP:HD1	1.63	0.63
2:B:191:LEU:HD21	2:B:214:VAL:HG21	1.81	0.63
1:O:97:THR:HG22	1:O:99:LEU:H	1.63	0.63
2:W:25:GLU:O	2:W:137:HIS:HE1	1.80	0.63
2:B:25:GLU:HA	2:B:41:CYS:HA	1.80	0.63
3:J:132:SER:HB2	3:J:155:ASN:HB3	1.81	0.63
3:X:134:PHE:HB2	3:X:153:LEU:HB3	1.80	0.63
2:B:49:PHE:HE1	2:B:54:MET:HE2	1.63	0.62
1:V:182:VAL:HG21	1:V:225:TYR:HB2	1.82	0.62
1:H:176:TYR:HB3	1:H:200:ALA:HB1	1.82	0.62
1:V:139:ASN:H	1:V:139:ASN:HD22	1.48	0.62
1:H:50:ARG:HE	1:H:52:MET:HE2	1.65	0.62
1:A:130:ASP:HB2	1:A:152:SER:HA	1.81	0.62
3:C:134:PHE:HB2	3:C:153:LEU:HB3	1.81	0.62
5:S:51:TRP:HE1	5:S:88:HIS:CE1	2.18	0.62
3:X:181:VAL:HG22	3:X:193:LEU:HD12	1.81	0.62
1:H:54:PHE:HB3	1:H:165:VAL:HG11	1.82	0.62
3:C:54:GLN:HB2	3:C:65:LEU:HD11	1.82	0.61
1:O:139:ASN:H	1:O:139:ASN:HD22	1.48	0.61
1:A:151:ILE:HD12	1:A:199:MET:HE1	1.82	0.61
2:P:36:ALA:HA	2:P:103:ASN:HA	1.83	0.61
1:O:176:TYR:HB3	1:O:200:ALA:HB1	1.81	0.61
4:K:68:ALA:HB1	4:K:89:ILE:HD13	1.81	0.61
2:P:39:LEU:HD12	2:P:100:LEU:HD23	1.83	0.61
1:V:54:PHE:HB3	1:V:165:VAL:HG11	1.83	0.61
1:A:147:ALA:HB2	3:C:109:ARG:NH2	2.15	0.61
1:H:139:ASN:HD22	1:H:139:ASN:H	1.48	0.61
1:O:169:LEU:HB2	1:O:232:ILE:HD13	1.83	0.61
2:I:200:ALA:HB1	2:I:208:TYR:HB3	1.82	0.61
7:G:67:TYR:HB3	7:G:70:LYS:HG3	1.82	0.61
4:D:117:LYS:HB3	4:D:133:ALA:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:39:LEU:HD12	2:W:100:LEU:HD23	1.83	0.60
2:B:79:TYR:HB2	2:B:84:LYS:HG3	1.83	0.60
1:V:151:ILE:HD11	1:V:208:TRP:HD1	1.63	0.60
1:V:215:LYS:NZ	1:V:265:GLU:HB3	2.16	0.60
1:A:316:LYS:HE2	1:A:318:GLU:HB2	1.83	0.60
2:I:39:LEU:HD12	2:I:100:LEU:HD23	1.82	0.60
3:C:181:VAL:HG22	3:C:193:LEU:HD12	1.82	0.60
2:W:200:ALA:HB1	2:W:208:TYR:HB3	1.83	0.60
6:T:59:ALA:HB3	6:T:62:LYS:HB2	1.83	0.60
2:W:36:ALA:HA	2:W:103:ASN:HA	1.83	0.60
1:H:97:THR:HG22	1:H:99:LEU:H	1.67	0.60
1:V:50:ARG:HE	1:V:52:MET:HE2	1.65	0.60
1:V:169:LEU:HB2	1:V:232:ILE:HD13	1.84	0.59
2:I:36:ALA:HA	2:I:103:ASN:HA	1.83	0.59
1:V:147:ALA:HB3	2:W:125:TRP:CH2	2.38	0.59
1:O:50:ARG:HE	1:O:52:MET:HE2	1.66	0.59
4:R:48:PHE:CE1	4:R:91:ARG:NH2	2.70	0.59
2:I:56:TRP:HD1	2:I:89:ILE:CD1	2.16	0.59
4:R:117:LYS:HB3	4:R:133:ALA:HB3	1.85	0.59
6:T:91:ARG:HH11	6:T:93:ASN:HD21	1.51	0.59
1:O:170:LYS:HD2	1:O:173:ASN:HA	1.85	0.59
1:O:110:ASP:HB3	1:O:113:GLU:HG3	1.85	0.59
5:E:24:LEU:HA	5:E:44:GLY:HA3	1.84	0.58
1:A:147:ALA:HB3	2:B:125:TRP:CH2	2.38	0.58
1:A:147:ALA:HB2	3:C:109:ARG:HH22	1.68	0.58
2:W:156:LEU:HD22	3:X:136:PHE:HB3	1.86	0.58
2:P:56:TRP:HD1	2:P:89:ILE:CD1	2.17	0.58
2:W:56:TRP:HD1	2:W:89:ILE:CD1	2.16	0.58
2:B:56:TRP:HD1	2:B:89:ILE:CD1	2.15	0.58
1:H:170:LYS:HZ2	1:H:173:ASN:H	1.51	0.58
1:V:215:LYS:HZ2	1:V:265:GLU:HB3	1.69	0.58
5:Z:84:PHE:HB3	6:a:81:PRO:HG2	1.86	0.57
1:V:176:TYR:HB3	1:V:200:ALA:HB1	1.86	0.57
1:H:169:LEU:HB2	1:H:232:ILE:HD13	1.85	0.57
7:b:40:ILE:HD12	7:b:90:LEU:HD23	1.85	0.57
1:H:182:VAL:HG21	1:H:225:TYR:HB2	1.87	0.57
4:R:110:THR:HG23	4:R:141:ILE:HA	1.87	0.56
1:O:31:ARG:HD2	1:O:360:ASN:HD21	1.70	0.56
2:B:79:TYR:CE1	2:B:89:ILE:HG22	2.40	0.56
7:G:24:LEU:HD21	7:G:45:SER:HB2	1.88	0.56
1:H:38:GLU:HB3	1:V:32:HIS:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:42:ILE:HG22	1:H:87:TRP:CD1	2.41	0.56
7:N:67:TYR:HB3	7:N:70:LYS:HG3	1.87	0.56
7:U:67:TYR:HB3	7:U:70:LYS:HG3	1.87	0.56
1:V:314:LEU:HG	1:V:316:LYS:NZ	2.20	0.56
1:H:31:ARG:HD2	1:H:360:ASN:HD21	1.71	0.56
6:M:23:LEU:HD23	6:M:43:ALA:HB2	1.87	0.56
1:V:42:ILE:HG22	1:V:87:TRP:CD1	2.40	0.56
1:A:139:ASN:HD22	1:A:139:ASN:H	1.51	0.56
2:B:127:TYR:CD1	3:C:113:GLY:HA2	2.41	0.56
3:C:132:SER:HB2	3:C:155:ASN:HB3	1.86	0.56
1:O:336:ASP:HB3	1:O:339:ARG:H	1.70	0.56
3:J:166:TRP:CD1	3:J:197:LEU:HD13	2.41	0.56
4:D:70:ILE:HB	4:D:89:ILE:HD12	1.87	0.56
6:F:127:ASP:OD1	6:F:131:GLU:OE2	2.24	0.56
6:a:110:THR:HG23	6:a:143:VAL:HG22	1.88	0.55
1:H:240:HIS:HE2	1:H:253:VAL:CG1	2.19	0.55
1:O:147:ALA:HB3	2:P:125:TRP:CH2	2.41	0.55
6:T:54:GLY:HA3	6:T:66:TYR:OH	2.06	0.55
6:T:91:ARG:HH11	6:T:93:ASN:ND2	2.02	0.55
6:T:37:LEU:HD23	6:T:105:LEU:HD21	1.89	0.55
1:V:336:ASP:HB3	1:V:339:ARG:H	1.71	0.55
1:A:122:GLU:HA	1:A:126:ASN:CB	2.37	0.55
6:F:37:LEU:HD23	6:F:105:LEU:HD21	1.88	0.55
1:O:215:LYS:NZ	1:O:265:GLU:HB3	2.21	0.55
1:H:230:PRO:HB3	1:H:239:PHE:CE1	2.42	0.55
1:A:132:THR:HG21	6:F:124:HIS:CE1	2.42	0.55
2:B:56:TRP:CD1	2:B:89:ILE:HD12	2.39	0.55
5:L:34:PRO:HA	5:L:95:VAL:HG12	1.89	0.55
1:A:134:HIS:HD2	1:A:136:PHE:CZ	2.25	0.55
1:H:215:LYS:HZ1	1:H:265:GLU:HB3	1.71	0.55
3:X:50:TYR:HE1	3:X:84:LYS:HE2	1.73	0.55
7:G:53:GLN:HG3	7:G:101:ALA:CB	2.36	0.54
1:V:36:ARG:HH11	1:V:38:GLU:HG3	1.71	0.54
1:A:42:ILE:HG22	1:A:87:TRP:CD1	2.42	0.54
1:A:245:ASP:O	1:A:248:ASN:O	2.25	0.54
3:C:49:TYR:HA	3:C:69:ASN:HD21	1.72	0.54
4:D:40:VAL:HG23	4:D:99:ARG:HG3	1.89	0.54
6:F:80:THR:HG22	6:F:83:VAL:HG22	1.90	0.54
7:b:103:TYR:HB2	7:b:119:THR:HG22	1.90	0.54
1:V:230:PRO:HB3	1:V:239:PHE:CE1	2.43	0.54
1:A:315:ILE:HG21	1:A:354:HIS:ND1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:216:TYR:CZ	1:H:218:ASN:HB3	2.42	0.54
7:N:38:VAL:HG11	7:N:121:LEU:HD21	1.90	0.54
1:A:56:TYR:CD2	1:A:114:ILE:HD11	2.43	0.54
4:K:126:THR:HG23	5:L:108:ARG:HE	1.73	0.54
1:O:240:HIS:HE2	1:O:253:VAL:CG1	2.20	0.53
2:B:81:ALA:HA	2:B:84:LYS:HE3	1.90	0.53
2:B:117:LYS:HB3	2:B:134:ALA:HB3	1.89	0.53
2:B:237:THR:HG22	2:B:239:VAL:HG23	1.91	0.53
6:T:127:ASP:OD1	6:T:131:GLU:OE2	2.26	0.53
3:C:43:SER:HB3	3:C:88:THR:HG22	1.89	0.53
6:M:54:GLY:HA3	6:M:66:TYR:OH	2.08	0.53
4:R:26:SER:HB3	4:R:40:VAL:HG12	1.90	0.53
1:O:126:ASN:ND2	6:T:72:ASN:HD21	2.06	0.53
6:F:54:GLY:HA3	6:F:66:TYR:OH	2.09	0.53
1:H:249:ASN:HD22	1:H:250:VAL:HG23	1.73	0.53
2:P:45:GLY:HA3	3:X:63:VAL:HG21	1.90	0.53
1:A:77:ILE:HD13	1:A:105:ILE:HD11	1.90	0.53
1:V:82:LYS:NZ	1:V:85:ASP:H	2.06	0.53
1:V:240:HIS:HE2	1:V:253:VAL:CG1	2.20	0.53
1:A:219:TYR:HA	1:A:225:TYR:OH	2.09	0.52
1:O:173:ASN:OD1	3:X:97:GLN:OE1	2.28	0.52
1:A:282:ASP:H	1:A:293:SER:HB3	1.74	0.52
1:H:275:LYS:HG2	1:H:278:LYS:HZ3	1.74	0.52
1:V:31:ARG:NH1	1:V:360:ASN:HD21	2.06	0.52
1:V:44:ASN:HB2	1:V:351:TYR:HE2	1.75	0.52
1:H:151:ILE:HD12	1:H:208:TRP:HD1	1.74	0.52
2:B:108:GLU:CD	2:B:108:GLU:H	2.18	0.52
1:H:130:ASP:HB3	1:H:152:SER:HA	1.90	0.52
1:A:119:CYS:HB3	1:A:131:MET:SD	2.50	0.52
1:H:240:HIS:NE2	1:H:253:VAL:HG11	2.23	0.52
6:M:37:LEU:HD13	6:M:39:LEU:HG	1.92	0.52
7:U:78:ARG:NH2	7:U:99:ASP:OD1	2.42	0.52
6:T:80:THR:HG22	6:T:83:VAL:HG22	1.92	0.52
2:B:56:TRP:CD1	2:B:89:ILE:CD1	2.93	0.52
1:H:45:ASN:ND2	4:K:121:SER:OG	2.43	0.52
7:N:100:GLU:HG3	7:N:183:GLN:HB3	1.91	0.52
1:H:31:ARG:HH11	1:H:360:ASN:HD21	1.57	0.51
1:H:147:ALA:HB3	2:I:125:TRP:CH2	2.45	0.51
1:A:182:VAL:HG21	1:A:225:TYR:HB2	1.92	0.51
4:D:110:THR:HG23	4:D:141:ILE:HA	1.92	0.51
1:H:44:ASN:HB2	1:H:351:TYR:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:202:ASP:HA	7:b:205:LYS:HD3	1.92	0.51
1:O:44:ASN:HB2	1:O:351:TYR:HE2	1.75	0.51
2:B:232:HIS:CD2	2:B:234:PRO:HD2	2.45	0.51
4:K:110:THR:HG23	4:K:141:ILE:HA	1.92	0.51
1:O:99:LEU:HD23	1:O:103:PRO:HB3	1.92	0.51
5:E:49:TYR:H	5:E:68:ASN:ND2	2.08	0.51
1:V:110:ASP:HB3	1:V:113:GLU:HG3	1.93	0.51
1:O:256:ILE:HG22	1:O:270:ASN:HA	1.93	0.51
2:B:41:CYS:HB3	2:B:98:LEU:HB3	1.91	0.51
2:B:176:ASP:HB3	2:B:207:LEU:HD22	1.91	0.51
3:J:88:THR:CG2	4:K:84:LYS:HD2	2.41	0.51
6:M:80:THR:HG22	6:M:83:VAL:HG22	1.92	0.51
1:A:107:ALA:HB2	1:A:116:ILE:HG23	1.93	0.51
1:A:336:ASP:HB3	1:A:339:ARG:H	1.76	0.51
1:H:151:ILE:HD11	1:H:208:TRP:CD1	2.45	0.51
1:V:84:LYS:O	1:V:85:ASP:HB2	2.11	0.51
3:X:131:PRO:HB3	3:X:157:PHE:HB3	1.93	0.51
5:E:108:ARG:HG2	5:E:112:ASN:O	2.11	0.51
7:G:53:GLN:HB2	7:G:103:TYR:CE2	2.46	0.51
2:B:30:LEU:HD22	2:B:179:PRO:HG3	1.92	0.50
1:H:52:MET:HE1	1:H:105:ILE:HB	1.91	0.50
1:A:54:PHE:HB3	1:A:165:VAL:HG11	1.93	0.50
1:A:56:TYR:CD2	1:A:57:LYS:HG2	2.46	0.50
3:J:38:VAL:HG12	3:J:93:ILE:HB	1.93	0.50
2:P:123:CYS:SG	3:Q:68:ASN:ND2	2.84	0.50
1:V:240:HIS:NE2	1:V:253:VAL:HG11	2.25	0.50
1:V:151:ILE:HD12	1:V:208:TRP:HD1	1.77	0.50
2:B:24:ASP:HB3	2:B:42:LYS:HB3	1.92	0.50
1:A:97:THR:HB	1:A:99:LEU:HB2	1.93	0.50
5:L:109:ASP:OD1	5:L:109:ASP:O	2.29	0.50
1:O:31:ARG:HH11	1:O:360:ASN:HD21	1.59	0.50
1:V:135:ARG:HB3	2:W:125:TRP:HH2	1.77	0.50
2:B:196:HIS:HE1	3:C:156:ASN:ND2	2.08	0.50
1:V:342:PHE:HB3	1:V:354:HIS:HB2	1.94	0.50
3:X:79:ARG:NH1	3:X:80:PHE:CE2	2.76	0.50
7:b:69:ASP:HB3	7:b:81:GLY:O	2.11	0.50
1:A:97:THR:C	1:A:99:LEU:H	2.19	0.50
3:J:54:GLN:HB2	3:J:65:LEU:HD11	1.94	0.50
1:V:245:ASP:O	1:V:248:ASN:O	2.30	0.50
2:I:203:GLN:HA	3:J:178:GLN:HE22	1.76	0.50
1:V:68:LEU:HB2	1:V:73:ASP:CB	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:68:LEU:HB2	1:O:73:ASP:HB3	1.93	0.49
1:V:256:ILE:HG22	1:V:270:ASN:HA	1.94	0.49
1:H:135:ARG:HB3	2:I:125:TRP:HH2	1.77	0.49
2:W:179:PRO:O	2:W:232:HIS:HE1	1.95	0.49
4:D:90:SER:HB3	4:D:99:ARG:HB2	1.94	0.49
6:M:86:ARG:NH2	6:M:109:ASP:OD2	2.30	0.49
1:A:135:ARG:HB3	2:B:125:TRP:CH2	2.48	0.49
3:X:38:VAL:HG12	3:X:93:ILE:HB	1.95	0.49
1:V:52:MET:HE1	1:V:105:ILE:HB	1.95	0.49
1:H:240:HIS:NE2	1:H:253:VAL:CG1	2.76	0.49
1:V:122:GLU:HG2	1:V:126:ASN:HB2	1.95	0.49
7:b:56:SER:HB2	7:b:59:SER:HB3	1.94	0.49
1:A:97:THR:C	1:A:99:LEU:N	2.71	0.49
1:A:117:LEU:CD2	1:A:149:ILE:HD11	2.43	0.49
1:H:110:ASP:HB3	1:H:113:GLU:HG2	1.95	0.49
1:H:233:SER:C	1:H:234:LYS:HG3	2.37	0.49
1:O:275:LYS:HG2	1:O:278:LYS:HZ3	1.77	0.49
4:R:59:ALA:HB3	4:R:62:LYS:HB2	1.94	0.49
5:S:109:ASP:OD1	5:S:109:ASP:O	2.31	0.49
1:A:77:ILE:HB	1:A:94:PHE:HB2	1.94	0.49
1:A:129:LYS:HB2	1:A:157:LYS:NZ	2.28	0.49
1:A:136:PHE:CD2	1:A:146:ASN:HB3	2.48	0.49
1:O:184:PRO:O	1:O:224:GLN:HA	2.12	0.49
1:O:240:HIS:NE2	1:O:253:VAL:HG11	2.25	0.49
1:A:195:ASP:HB3	1:A:219:TYR:CD2	2.47	0.48
1:A:229:ARG:HH12	1:A:231:TYR:HB2	1.77	0.48
2:I:117:LYS:HB3	2:I:134:ALA:HB3	1.94	0.48
1:O:342:PHE:HB3	1:O:354:HIS:HB2	1.94	0.48
1:V:240:HIS:NE2	1:V:253:VAL:CG1	2.76	0.48
1:H:240:HIS:CD2	1:H:253:VAL:CG1	2.96	0.48
3:Q:38:VAL:HG12	3:Q:93:ILE:HB	1.96	0.48
3:X:69:ASN:HD21	3:X:84:LYS:HD2	1.79	0.48
1:H:167:LEU:HB2	1:H:168:PRO:HD2	1.95	0.48
1:O:167:LEU:HB2	1:O:168:PRO:HD2	1.95	0.48
7:U:78:ARG:HH21	7:U:99:ASP:CG	2.21	0.48
1:V:135:ARG:HB3	2:W:125:TRP:CH2	2.47	0.48
1:A:115:ILE:HD13	1:A:177:PHE:CE2	2.49	0.48
1:A:132:THR:CG2	6:F:124:HIS:CE1	2.97	0.48
3:C:85:SER:HB3	4:D:84:LYS:HD3	1.96	0.48
4:D:59:ALA:HB3	4:D:62:LYS:HB2	1.95	0.48
2:W:151:PRO:HD2	2:W:237:THR:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:110:THR:HG23	4:Y:141:ILE:HA	1.94	0.48
6:a:37:LEU:HD21	6:a:102:LEU:HB3	1.96	0.48
3:J:103:VAL:HG22	3:J:121:THR:HG22	1.95	0.48
4:K:59:ALA:HB3	4:K:62:LYS:HB2	1.95	0.48
4:K:117:LYS:HB3	4:K:133:ALA:HB3	1.96	0.48
4:K:90:SER:HB3	4:K:99:ARG:HB2	1.96	0.48
1:A:70:GLY:H	1:A:73:ASP:HB2	1.78	0.48
1:H:256:ILE:HG22	1:H:270:ASN:HA	1.95	0.48
1:O:151:ILE:HD12	1:O:208:TRP:HD1	1.77	0.48
4:R:69:ASP:OD1	4:R:69:ASP:O	2.31	0.48
4:Y:90:SER:HB3	4:Y:99:ARG:HB2	1.95	0.48
1:H:174:ARG:NH1	1:H:202:HIS:CD2	2.75	0.48
1:H:261:GLU:HB2	1:H:267:VAL:HG12	1.95	0.48
5:Z:49:TYR:OH	5:Z:86:SER:O	2.31	0.48
7:b:67:TYR:HB3	7:b:70:LYS:HG3	1.95	0.48
1:A:36:ARG:HG3	1:O:34:PHE:CD1	2.48	0.48
1:A:129:LYS:HB2	1:A:157:LYS:HZ2	1.79	0.48
1:A:99:LEU:HD12	1:A:103:PRO:HB3	1.96	0.48
2:B:25:GLU:O	2:B:25:GLU:HG2	2.13	0.48
4:D:55:TRP:HE1	4:D:98:VAL:HG12	1.79	0.48
1:V:167:LEU:HB2	1:V:168:PRO:HD2	1.95	0.48
1:A:283:VAL:HG22	1:A:292:VAL:HG12	1.95	0.47
6:F:59:ALA:HB3	6:F:62:LYS:HB2	1.96	0.47
1:O:240:HIS:CD2	1:O:253:VAL:CG1	2.97	0.47
4:R:90:SER:HB3	4:R:99:ARG:HB2	1.95	0.47
1:V:42:ILE:CG2	1:V:87:TRP:CD1	2.96	0.47
1:A:295:GLY:HA3	1:A:300:PHE:CD1	2.49	0.47
1:H:126:ASN:HD21	6:M:72:ASN:HD21	1.60	0.47
1:H:151:ILE:CD1	1:H:208:TRP:CD1	2.92	0.47
6:M:232:HIS:ND1	6:M:235:SER:OG	2.44	0.47
1:O:205:GLY:HA2	1:O:208:TRP:CZ2	2.49	0.47
1:O:240:HIS:NE2	1:O:253:VAL:CG1	2.77	0.47
1:V:205:GLY:HA2	1:V:208:TRP:CZ2	2.50	0.47
5:E:37:THR:HG22	5:E:93:THR:HA	1.95	0.47
2:W:117:LYS:HB3	2:W:134:ALA:HB3	1.96	0.47
3:X:73:PRO:HG2	3:X:76:ILE:HG13	1.97	0.47
1:H:42:ILE:CG2	1:H:87:TRP:CD1	2.97	0.47
6:M:107:ALA:HA	6:M:143:VAL:HG21	1.95	0.47
1:V:56:TYR:HB3	1:V:61:TYR:CE2	2.50	0.47
1:A:42:ILE:CG2	1:A:87:TRP:CD1	2.97	0.47
1:H:342:PHE:HB3	1:H:354:HIS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:182:VAL:HG23	1:O:196:ILE:HG12	1.97	0.47
3:J:88:THR:HG21	4:K:84:LYS:HD2	1.95	0.47
4:Y:53:MET:HE1	4:Y:117:LYS:HG3	1.95	0.47
7:b:71:ARG:NH1	7:b:75:ILE:O	2.47	0.47
1:A:147:ALA:HB3	2:B:125:TRP:CZ2	2.50	0.47
2:B:79:TYR:HE1	2:B:89:ILE:HG22	1.80	0.47
1:H:135:ARG:HB3	2:I:125:TRP:CH2	2.50	0.47
1:O:282:ASP:H	1:O:293:SER:HB3	1.79	0.47
4:R:91:ARG:HD3	4:R:93:ASP:OD1	2.15	0.47
3:X:54:GLN:HG3	3:X:104:TYR:CE2	2.50	0.47
1:A:315:ILE:CG2	1:A:354:HIS:ND1	2.78	0.47
6:M:59:ALA:HB3	6:M:62:LYS:HB2	1.97	0.47
1:O:37:THR:HG21	1:O:313:ILE:HD13	1.98	0.47
1:O:273:PHE:HB2	1:O:280:LEU:HD22	1.96	0.47
2:P:36:ALA:HB1	2:P:101:GLN:HE22	1.79	0.47
1:V:240:HIS:CD2	1:V:253:VAL:CG1	2.97	0.47
1:A:42:ILE:HB	1:A:351:TYR:HB2	1.97	0.46
1:A:134:HIS:CD2	1:A:136:PHE:CZ	3.04	0.46
2:B:196:HIS:CE1	3:C:156:ASN:HD21	2.29	0.46
4:K:26:SER:HB3	4:K:40:VAL:HG12	1.97	0.46
1:O:56:TYR:HB3	1:O:61:TYR:CE2	2.50	0.46
2:P:117:LYS:HB3	2:P:134:ALA:HB3	1.97	0.46
2:I:36:ALA:HB1	2:I:101:GLN:HE22	1.80	0.46
2:I:176:ASP:HB3	2:I:207:LEU:HD22	1.96	0.46
5:Z:39:LYS:HB2	5:Z:39:LYS:HE2	1.77	0.46
5:Z:102:VAL:HG22	5:Z:120:THR:HG23	1.98	0.46
4:R:55:TRP:HE1	4:R:98:VAL:HG12	1.80	0.46
2:I:149:LYS:HE2	2:I:207:LEU:HD21	1.98	0.46
4:K:53:MET:HE1	4:K:117:LYS:HG3	1.98	0.46
1:H:56:TYR:HB3	1:H:61:TYR:CE2	2.51	0.46
3:J:73:PRO:HG2	3:J:76:ILE:HG13	1.97	0.46
1:O:275:LYS:HG2	1:O:278:LYS:NZ	2.31	0.46
1:V:151:ILE:HD11	1:V:208:TRP:CD1	2.46	0.46
4:D:70:ILE:HG12	4:D:91:ARG:HG2	1.98	0.46
1:O:151:ILE:HD11	1:O:208:TRP:CD1	2.44	0.46
1:O:228:LEU:HA	1:O:241:PHE:HB3	1.98	0.46
2:P:42:LYS:HD2	2:P:97:THR:HG23	1.98	0.46
1:V:282:ASP:H	1:V:293:SER:HB3	1.81	0.46
6:F:70:ILE:HG23	6:F:91:ARG:HH21	1.79	0.46
6:F:129:SER:O	7:G:106:GLY:HA3	2.16	0.46
2:W:176:ASP:HB3	2:W:207:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:THR:HG23	2:B:212:SER:HB2	1.98	0.46
1:H:282:ASP:H	1:H:293:SER:HB3	1.81	0.46
2:W:53:THR:HG23	2:W:118:HIS:CB	2.46	0.46
2:B:84:LYS:HE3	2:B:84:LYS:HB2	1.72	0.46
2:I:203:GLN:NE2	2:I:209:SER:HB3	2.31	0.46
4:K:91:ARG:HD3	4:K:93:ASP:OD1	2.16	0.46
1:O:174:ARG:NH1	1:O:202:HIS:CD2	2.76	0.46
3:X:142:GLN:HE22	3:X:149:SER:HB2	1.80	0.46
3:C:228:ASN:O	3:C:229:ARG:HD3	2.16	0.45
1:H:205:GLY:HA2	1:H:208:TRP:CZ2	2.51	0.45
1:H:275:LYS:HG2	1:H:278:LYS:NZ	2.31	0.45
1:O:151:ILE:CD1	1:O:208:TRP:CD1	2.93	0.45
1:V:253:VAL:HG12	1:V:254:ASN:H	1.82	0.45
2:I:56:TRP:HD1	2:I:89:ILE:HD12	1.81	0.45
3:J:166:TRP:CG	3:J:197:LEU:HD13	2.51	0.45
4:K:70:ILE:HB	4:K:89:ILE:HD12	1.99	0.45
6:M:76:PHE:HE2	6:M:78:LEU:HD23	1.81	0.45
2:B:25:GLU:O	2:B:137:HIS:CE1	2.69	0.45
1:A:174:ARG:CZ	1:A:202:HIS:HD2	2.30	0.45
1:A:311:ASN:HA	1:O:312:SER:O	2.15	0.45
4:D:40:VAL:HG22	4:D:97:THR:HB	1.99	0.45
1:O:52:MET:HE1	1:O:105:ILE:HB	1.98	0.45
3:Q:63:VAL:HG21	2:W:45:GLY:HA3	1.98	0.45
1:V:273:PHE:HB2	1:V:280:LEU:HD22	1.97	0.45
6:a:129:SER:HB3	7:b:113:VAL:CG1	2.47	0.45
3:C:73:PRO:HG2	3:C:76:ILE:HG13	1.99	0.45
7:G:35:GLY:O	7:G:94:GLY:HA2	2.17	0.45
1:V:315:ILE:HG21	1:V:354:HIS:CD2	2.52	0.45
2:W:42:LYS:HD2	2:W:97:THR:HG23	1.99	0.45
2:B:137:HIS:H	2:B:137:HIS:CD2	2.34	0.45
2:B:197:THR:HA	2:B:212:SER:HA	1.99	0.45
1:H:273:PHE:HB2	1:H:280:LEU:HD22	1.99	0.45
2:I:53:THR:HG23	2:I:118:HIS:CB	2.47	0.45
2:I:58:ARG:HG2	2:I:68:VAL:CG2	2.46	0.45
1:A:39:LEU:HD21	1:A:354:HIS:CE1	2.51	0.45
3:J:50:TYR:HE1	3:J:84:LYS:HE2	1.82	0.45
3:J:87:SER:OG	5:L:112:ASN:ND2	2.50	0.45
4:K:36:THR:HG22	4:K:103:ASN:HB3	1.99	0.45
1:V:82:LYS:HZ2	1:V:85:ASP:H	1.65	0.45
1:A:230:PRO:HB3	1:A:239:PHE:CE1	2.52	0.45
1:V:104:HIS:NE2	1:V:121:ASP:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:117:LYS:HB3	4:Y:133:ALA:HB3	1.99	0.45
2:B:198:PHE:CZ	3:C:192:SER:HB3	2.51	0.44
5:E:78:ARG:HH21	5:E:96:GLN:HE22	1.65	0.44
1:H:253:VAL:HG12	1:H:254:ASN:H	1.82	0.44
1:H:322:ASN:HB3	1:H:325:ALA:CB	2.46	0.44
1:V:170:LYS:HE2	1:V:173:ASN:HA	1.99	0.44
4:Y:91:ARG:HD3	4:Y:93:ASP:OD1	2.17	0.44
1:A:295:GLY:HA3	1:A:300:PHE:HD1	1.82	0.44
1:A:348:GLN:HE21	1:A:349:GLY:H	1.64	0.44
4:D:83:VAL:HB	4:D:87:ALA:HB2	1.99	0.44
5:L:49:TYR:CD2	5:L:88:HIS:HB2	2.51	0.44
1:A:242:TYR:HB3	1:A:251:LYS:HB2	2.00	0.44
2:B:24:ASP:HA	2:B:137:HIS:NE2	2.32	0.44
4:K:126:THR:CG2	5:L:108:ARG:HE	2.29	0.44
1:O:135:ARG:HB3	2:P:125:TRP:HH2	1.82	0.44
1:O:322:ASN:HB3	1:O:325:ALA:HB2	1.99	0.44
2:P:53:THR:HG23	2:P:118:HIS:CB	2.47	0.44
3:Q:73:PRO:HG2	3:Q:76:ILE:HG13	1.98	0.44
6:T:129:SER:O	7:U:106:GLY:HA3	2.16	0.44
2:W:58:ARG:HG2	2:W:68:VAL:CG2	2.47	0.44
2:B:185:SER:O	2:B:229:ASN:CB	2.63	0.44
1:H:253:VAL:HG12	1:H:254:ASN:N	2.33	0.44
4:R:79:TYR:HE1	4:R:89:ILE:HG12	1.83	0.44
1:V:71:GLU:H	1:V:71:GLU:HG3	1.56	0.44
2:W:106:ARG:HD3	2:W:108:GLU:HB2	1.99	0.44
1:A:97:THR:HG23	1:A:134:HIS:CD2	2.52	0.44
2:B:108:GLU:CD	2:B:108:GLU:N	2.75	0.44
6:T:129:SER:HB3	7:U:113:VAL:CG1	2.48	0.44
1:V:216:TYR:CE1	1:V:218:ASN:HB2	2.53	0.44
2:W:36:ALA:HB1	2:W:101:GLN:HE22	1.83	0.44
6:a:54:GLY:HA3	6:a:66:TYR:OH	2.17	0.44
1:A:89:THR:HB	4:D:123:TYR:HA	2.00	0.44
1:O:245:ASP:O	1:O:248:ASN:O	2.36	0.44
1:A:39:LEU:CD2	1:A:354:HIS:CD2	2.97	0.44
3:C:63:VAL:HG21	2:I:45:GLY:HA3	1.98	0.44
4:D:36:THR:HG22	4:D:103:ASN:HB3	2.00	0.44
4:D:67:VAL:HG13	4:D:83:VAL:HG21	2.00	0.44
1:V:31:ARG:HH11	1:V:360:ASN:HD21	1.65	0.44
1:A:174:ARG:HD2	1:A:202:HIS:HB2	2.00	0.44
3:C:142:GLN:HE22	3:C:149:SER:HB2	1.82	0.44
1:H:39:LEU:HG	1:H:354:HIS:HE1	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:52:TYR:HE2	2:I:117:LYS:HZ3	1.65	0.44
4:K:40:VAL:HG23	4:K:99:ARG:HG3	1.99	0.44
1:O:138:SER:OG	1:O:143:GLU:O	2.29	0.44
1:V:138:SER:OG	1:V:143:GLU:O	2.29	0.43
1:A:42:ILE:HD11	1:A:82:LYS:HD2	2.00	0.43
6:F:76:PHE:HE2	6:F:78:LEU:HD23	1.83	0.43
1:O:316:LYS:O	1:O:319:LYS:HG2	2.18	0.43
4:R:36:THR:HG22	4:R:103:ASN:HB3	1.99	0.43
4:Y:36:THR:HG22	4:Y:103:ASN:HB3	2.00	0.43
1:A:273:PHE:HB2	1:A:280:LEU:HD22	1.99	0.43
4:D:39:LEU:HB2	4:D:100:LEU:HB3	2.00	0.43
7:G:100:GLU:O	7:G:101:ALA:HB2	2.18	0.43
1:O:253:VAL:HG12	1:O:254:ASN:N	2.34	0.43
1:A:260:HIS:HE1	1:A:264:LEU:H	1.66	0.43
1:H:347:SER:HB3	1:H:350:ILE:HB	2.01	0.43
4:K:66:TRP:HB2	4:K:128:LEU:HD11	2.00	0.43
1:V:253:VAL:HG12	1:V:254:ASN:N	2.32	0.43
2:B:25:GLU:OE2	2:B:136:GLY:HA3	2.18	0.43
2:I:22:THR:HB	2:I:44:SER:HB2	2.01	0.43
1:O:253:VAL:HG12	1:O:254:ASN:H	1.83	0.43
6:T:49:SER:HA	6:T:93:ASN:HD22	1.82	0.43
1:A:122:GLU:C	1:A:126:ASN:HB2	2.42	0.43
1:A:122:GLU:CA	1:A:126:ASN:HB2	2.43	0.43
1:A:126:ASN:HD22	1:A:126:ASN:HA	1.78	0.43
2:B:151:PRO:HB3	2:B:177:TYR:HB3	2.01	0.43
3:C:65:LEU:O	3:C:73:PRO:HD2	2.18	0.43
6:F:22:THR:OG1	6:F:44:SER:OG	2.37	0.43
1:V:151:ILE:CD1	1:V:208:TRP:CD1	2.94	0.43
1:O:316:LYS:HE2	1:O:316:LYS:HB2	1.57	0.43
1:A:91:ASN:OD1	1:A:93:LEU:HG	2.18	0.43
1:A:99:LEU:O	7:G:111:ARG:NH1	2.52	0.43
1:A:104:HIS:O	1:A:118:LEU:HA	2.18	0.43
1:A:117:LEU:HG	1:A:134:HIS:O	2.19	0.43
2:I:53:THR:HB	2:I:72:SER:HA	2.01	0.43
2:P:22:THR:HB	2:P:44:SER:HB2	2.01	0.43
4:R:39:LEU:HB2	4:R:100:LEU:HB3	2.00	0.43
2:W:56:TRP:HD1	2:W:89:ILE:HD11	1.84	0.43
1:A:340:ALA:O	1:A:356:ILE:HB	2.18	0.43
2:P:53:THR:HB	2:P:72:SER:HA	2.01	0.43
1:V:36:ARG:HB3	1:V:357:TYR:HB3	2.00	0.43
1:A:167:LEU:HB2	1:A:168:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:41:CYS:SG	4:D:55:TRP:CZ2	3.12	0.42
1:H:218:ASN:HA	1:H:220:LYS:NZ	2.34	0.42
3:Q:65:LEU:O	3:Q:73:PRO:HD2	2.18	0.42
6:T:22:THR:OG1	6:T:44:SER:OG	2.37	0.42
4:Y:26:SER:HB3	4:Y:40:VAL:HG12	2.01	0.42
5:Z:108:ARG:HA	5:Z:113:GLY:HA2	2.01	0.42
7:b:51:TRP:CZ3	7:b:105:CYS:HB3	2.54	0.42
7:U:32:ALA:HB3	7:U:38:VAL:HG22	2.01	0.42
2:W:22:THR:HB	2:W:44:SER:HB2	2.01	0.42
5:Z:48:ASP:O	5:Z:107:SER:OG	2.33	0.42
1:A:151:ILE:HD12	1:A:199:MET:CE	2.48	0.42
1:H:88:ILE:HG21	4:K:71:CYS:SG	2.59	0.42
1:V:50:ARG:NE	1:V:52:MET:HE2	2.33	0.42
1:V:292:VAL:HG23	1:V:306:PHE:HB2	2.01	0.42
5:Z:51:TRP:NE1	5:Z:88:HIS:CE1	2.85	0.42
1:H:50:ARG:NE	1:H:52:MET:HE2	2.32	0.42
5:S:42:CYS:HB2	5:S:51:TRP:CZ2	2.54	0.42
4:Y:79:TYR:HE1	4:Y:89:ILE:HG12	1.84	0.42
1:A:115:ILE:HD13	1:A:177:PHE:CZ	2.54	0.42
4:Y:39:LEU:HB2	4:Y:100:LEU:HB3	2.00	0.42
5:Z:60:ALA:HA	5:Z:61:PRO:HD3	1.94	0.42
7:N:33:ASN:HA	7:N:124:LEU:HB2	2.01	0.42
7:N:166:LYS:HB2	7:N:210:ALA:HB3	2.01	0.42
1:O:39:LEU:HG	1:O:354:HIS:HE1	1.79	0.42
1:V:315:ILE:CG2	1:V:354:HIS:CE1	3.03	0.42
1:A:319:LYS:HD3	1:A:319:LYS:HA	1.88	0.42
2:I:237:THR:HG22	2:I:239:VAL:HG23	2.01	0.42
2:P:56:TRP:HD1	2:P:89:ILE:HD12	1.83	0.42
7:U:125:ARG:CD	7:U:188:SER:HB2	2.50	0.42
1:A:95:LYS:O	1:A:95:LYS:CG	2.66	0.42
2:W:53:THR:HB	2:W:72:SER:HA	2.02	0.42
1:A:103:PRO:HB2	1:A:118:LEU:HB3	2.02	0.42
1:A:128:LYS:HE2	1:A:128:LYS:HB3	1.71	0.42
1:H:215:LYS:NZ	1:H:265:GLU:HB3	2.35	0.42
3:J:79:ARG:NH1	3:J:80:PHE:CE1	2.74	0.42
7:N:40:ILE:O	7:N:89:THR:HA	2.20	0.42
2:W:56:TRP:HD1	2:W:89:ILE:HD12	1.82	0.42
6:a:24:ASP:HA	6:a:137:HIS:NE2	2.35	0.42
1:O:36:ARG:HB3	1:O:357:TYR:HB3	2.02	0.42
1:O:135:ARG:HB3	2:P:125:TRP:CH2	2.54	0.42
7:U:125:ARG:HH21	7:U:128:ALA:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ASN:HB2	1:A:87:TRP:HD1	1.84	0.41
3:J:168:VAL:CG1	3:J:207:HIS:ND1	2.83	0.41
7:N:98:GLU:CD	7:N:98:GLU:H	2.27	0.41
3:C:49:TYR:HA	3:C:69:ASN:ND2	2.34	0.41
4:R:116:ALA:HB1	4:R:131:ILE:HG23	2.01	0.41
7:U:33:ASN:HA	7:U:124:LEU:HB2	2.02	0.41
4:D:79:TYR:HE1	4:D:89:ILE:HG12	1.85	0.41
1:O:210:THR:HG23	1:O:264:LEU:HD21	2.03	0.41
1:O:215:LYS:HZ1	1:O:265:GLU:HB3	1.84	0.41
2:P:29:GLY:O	2:P:31:GLN:HG2	2.20	0.41
4:R:66:TRP:HB2	4:R:128:LEU:HD11	2.01	0.41
6:T:91:ARG:NH1	6:T:93:ASN:HD21	2.15	0.41
1:V:273:PHE:O	1:V:294:TYR:OH	2.30	0.41
2:W:130:GLY:C	2:W:131:CYS:SG	3.03	0.41
1:A:278:LYS:NZ	1:A:278:LYS:HB2	2.35	0.41
3:C:30:VAL:HG12	3:C:120:THR:HG22	2.03	0.41
5:S:32:ALA:HB3	5:S:38:VAL:HG22	2.01	0.41
1:V:159:LYS:HE2	1:V:183:SER:HB2	2.03	0.41
7:b:54:GLN:HB2	7:b:61:PRO:HB3	2.02	0.41
2:I:56:TRP:CD1	2:I:89:ILE:HD11	2.56	0.41
1:O:347:SER:HB3	1:O:350:ILE:HB	2.02	0.41
7:U:166:LYS:HB2	7:U:210:ALA:HB3	2.02	0.41
2:B:25:GLU:HB3	2:B:115:CYS:HB2	2.02	0.41
5:E:51:TRP:NE1	5:E:88:HIS:CE1	2.86	0.41
1:H:186:LYS:HG3	1:H:221:LEU:CD2	2.50	0.41
1:H:229:ARG:HA	1:H:230:PRO:HD3	1.91	0.41
2:I:54:MET:HB3	2:I:98:LEU:HD22	2.02	0.41
6:M:157:ALA:HA	6:M:158:PRO:HD3	1.96	0.41
7:N:125:ARG:HD2	7:N:126:THR:H	1.86	0.41
5:S:85:GLY:HA2	7:U:109:ASP:O	2.20	0.41
2:W:29:GLY:O	2:W:31:GLN:HG2	2.21	0.41
2:W:124:ASP:HB3	3:X:48:SER:HB2	2.02	0.41
3:X:152:CYS:HB2	3:X:166:TRP:CH2	2.55	0.41
7:G:45:SER:OG	7:G:108:SER:O	2.36	0.41
7:G:64:VAL:HG12	7:G:65:ILE:HG12	2.03	0.41
3:X:110:ASP:HB2	3:X:115:ILE:CG2	2.51	0.41
1:A:151:ILE:H	1:A:151:ILE:HG12	1.56	0.41
2:B:179:PRO:HD2	2:B:234:PRO:HG2	2.01	0.41
6:M:37:LEU:HD23	6:M:105:LEU:HD21	2.03	0.41
2:P:56:TRP:CD1	2:P:89:ILE:HD11	2.56	0.41
2:P:106:ARG:HE	2:P:108:GLU:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:38:VAL:HG11	5:S:121:LEU:CD1	2.50	0.41
2:W:87:ALA:HB2	2:W:102:LEU:HD13	2.03	0.41
5:Z:31:SER:HB2	5:Z:124:LEU:HD13	2.03	0.41
1:A:52:MET:O	1:A:62:ASN:HA	2.20	0.41
2:B:110:THR:HG23	2:B:142:ILE:HA	2.03	0.41
2:I:151:PRO:HD2	2:I:237:THR:HG21	2.02	0.41
3:J:30:VAL:HG12	3:J:120:THR:HG22	2.03	0.41
6:M:79:TYR:CE1	6:M:89:ILE:HG22	2.56	0.41
1:O:97:THR:HG22	1:O:98:ASP:N	2.36	0.41
1:O:242:TYR:CE2	1:O:253:VAL:HG22	2.55	0.41
1:O:292:VAL:HG23	1:O:306:PHE:HB2	2.02	0.41
2:P:32:THR:HA	2:P:33:PRO:HD3	1.96	0.41
4:R:48:PHE:CD1	4:R:91:ARG:NH2	2.87	0.41
1:V:322:ASN:HB3	1:V:325:ALA:CB	2.45	0.41
1:V:347:SER:HB3	1:V:350:ILE:HB	2.01	0.41
2:W:56:TRP:CD1	2:W:89:ILE:HD11	2.55	0.41
3:X:203:ASP:HA	3:X:206:LYS:HE3	2.02	0.41
1:A:32:HIS:HD2	1:O:38:GLU:HB3	1.86	0.41
1:A:79:VAL:CG2	1:A:93:LEU:HD21	2.51	0.41
1:A:99:LEU:CD1	1:A:103:PRO:HB3	2.51	0.41
1:H:228:LEU:HD21	1:H:239:PHE:CD1	2.55	0.41
2:I:32:THR:HA	2:I:33:PRO:HD3	1.97	0.41
6:M:70:ILE:HG23	6:M:91:ARG:HH21	1.86	0.41
6:M:116:THR:HB	6:M:132:ILE:HG21	2.02	0.41
1:H:63:ILE:HG21	1:H:105:ILE:HG21	2.03	0.40
2:I:127:TYR:CD1	3:J:113:GLY:HA2	2.57	0.40
1:O:50:ARG:NE	1:O:52:MET:HE2	2.34	0.40
6:a:80:THR:HG22	6:a:83:VAL:H	1.86	0.40
1:A:98:ASP:OD1	6:F:125:TYR:HB2	2.20	0.40
7:G:23:ALA:HA	7:G:109:ASP:OD2	2.21	0.40
7:N:27:PRO:O	7:N:119:THR:OG1	2.34	0.40
1:O:216:TYR:CE1	1:O:218:ASN:HB2	2.56	0.40
4:R:53:MET:HE1	4:R:117:LYS:HG3	2.01	0.40
1:H:95:LYS:NZ	5:L:48:ASP:CG	2.80	0.40
1:H:242:TYR:CE2	1:H:253:VAL:HG22	2.56	0.40
3:J:110:ASP:HB2	3:J:115:ILE:CG2	2.51	0.40
1:O:316:LYS:HA	1:O:317:PRO:HD3	1.90	0.40
1:O:327:CYS:HA	1:O:344:TYR:CD2	2.56	0.40
1:V:39:LEU:HG	1:V:354:HIS:HE1	1.79	0.40
1:A:83:VAL:HG11	4:D:73:GLY:HA3	2.02	0.40
1:A:132:THR:CG2	6:F:124:HIS:NE2	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:THR:O	1:A:334:LYS:HD2	2.21	0.40
6:T:79:TYR:CE1	6:T:89:ILE:HG22	2.56	0.40
1:V:242:TYR:CE2	1:V:253:VAL:HG22	2.56	0.40
1:V:251:LYS:HB2	1:V:251:LYS:HE3	1.92	0.40
3:X:166:TRP:HB2	3:X:173:GLN:HB2	2.03	0.40
4:Y:83:VAL:HA	4:Y:86:ARG:HH11	1.86	0.40
2:B:52:TYR:CE2	2:B:117:LYS:NZ	2.89	0.40
2:B:124:ASP:HB3	3:C:48:SER:HB2	2.03	0.40
2:I:30:LEU:HD22	2:I:179:PRO:HG3	2.03	0.40
1:O:317:PRO:C	1:O:319:LYS:H	2.30	0.40
2:P:58:ARG:HG2	2:P:68:VAL:CG2	2.52	0.40
1:V:315:ILE:HG22	1:V:354:HIS:CE1	2.57	0.40
2:W:148:THR:HG22	2:W:235:SER:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/343 (94%)	267 (82%)	57 (18%)	0	100	100
1	H	313/343 (91%)	283 (90%)	30 (10%)	0	100	100
1	O	323/343 (94%)	295 (91%)	28 (9%)	0	100	100
1	V	321/343 (94%)	289 (90%)	32 (10%)	0	100	100
2	B	217/230 (94%)	202 (93%)	15 (7%)	0	100	100
2	I	217/230 (94%)	198 (91%)	19 (9%)	0	100	100
2	P	217/230 (94%)	202 (93%)	15 (7%)	0	100	100
2	W	214/230 (93%)	193 (90%)	21 (10%)	0	100	100
3	C	205/210 (98%)	189 (92%)	16 (8%)	0	100	100
3	J	205/210 (98%)	191 (93%)	14 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	205/210 (98%)	189 (92%)	16 (8%)	0	100	100
3	X	204/210 (97%)	190 (93%)	14 (7%)	0	100	100
4	D	217/230 (94%)	210 (97%)	7 (3%)	0	100	100
4	K	216/230 (94%)	207 (96%)	9 (4%)	0	100	100
4	R	217/230 (94%)	212 (98%)	5 (2%)	0	100	100
4	Y	217/230 (94%)	210 (97%)	7 (3%)	0	100	100
5	E	200/209 (96%)	190 (95%)	10 (5%)	0	100	100
5	L	199/209 (95%)	191 (96%)	8 (4%)	0	100	100
5	S	196/209 (94%)	187 (95%)	9 (5%)	0	100	100
5	Z	199/209 (95%)	190 (96%)	9 (4%)	0	100	100
6	F	219/321 (68%)	205 (94%)	14 (6%)	0	100	100
6	M	219/321 (68%)	203 (93%)	16 (7%)	0	100	100
6	T	214/321 (67%)	201 (94%)	13 (6%)	0	100	100
6	a	215/321 (67%)	195 (91%)	20 (9%)	0	100	100
7	G	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
7	N	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
7	U	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
7	b	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
All	All	6319/7008 (90%)	5874 (93%)	445 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/316 (97%)	250 (82%)	56 (18%)	2	7
1	H	300/316 (95%)	253 (84%)	47 (16%)	2	11
1	O	305/316 (96%)	256 (84%)	49 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	303/316 (96%)	250 (82%)	53 (18%)	2	8
2	B	177/186 (95%)	159 (90%)	18 (10%)	7	25
2	I	177/186 (95%)	163 (92%)	14 (8%)	11	35
2	P	177/186 (95%)	164 (93%)	13 (7%)	13	38
2	W	176/186 (95%)	162 (92%)	14 (8%)	11	35
3	C	177/179 (99%)	157 (89%)	20 (11%)	5	22
3	J	177/179 (99%)	161 (91%)	16 (9%)	9	30
3	Q	177/179 (99%)	156 (88%)	21 (12%)	5	20
3	X	177/179 (99%)	153 (86%)	24 (14%)	3	16
4	D	179/188 (95%)	156 (87%)	23 (13%)	4	18
4	K	179/188 (95%)	158 (88%)	21 (12%)	5	21
4	R	179/188 (95%)	155 (87%)	24 (13%)	4	16
4	Y	179/188 (95%)	153 (86%)	26 (14%)	3	14
5	E	175/179 (98%)	159 (91%)	16 (9%)	9	30
5	L	175/179 (98%)	154 (88%)	21 (12%)	5	20
5	S	173/179 (97%)	156 (90%)	17 (10%)	7	27
5	Z	175/179 (98%)	157 (90%)	18 (10%)	7	25
6	F	179/272 (66%)	165 (92%)	14 (8%)	11	36
6	M	179/272 (66%)	161 (90%)	18 (10%)	7	26
6	T	176/272 (65%)	159 (90%)	17 (10%)	8	27
6	a	176/272 (65%)	159 (90%)	17 (10%)	8	27
7	G	180/180 (100%)	167 (93%)	13 (7%)	13	39
7	N	180/180 (100%)	163 (91%)	17 (9%)	8	29
7	U	180/180 (100%)	165 (92%)	15 (8%)	10	34
7	b	179/180 (99%)	146 (82%)	33 (18%)	1	7
All	All	5472/6000 (91%)	4817 (88%)	655 (12%)	5	20

All (655) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	39	LEU
1	A	50	ARG

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Mol	Chain	Res	Type
1	A	52	MET
1	A	59	GLU
1	A	63	ILE
1	A	69	LYS
1	A	81	LYS
1	A	91	ASN
1	A	93	LEU
1	A	95	LYS
1	A	97	THR
1	A	99	LEU
1	A	100	THR
1	A	111	VAL
1	A	114	ILE
1	A	121	ASP
1	A	125	SER
1	A	128	LYS
1	A	129	LYS
1	A	132	THR
1	A	133	CYS
1	A	134	HIS
1	A	139	ASN
1	A	143	GLU
1	A	145	ASN
1	A	146	ASN
1	A	151	ILE
1	A	152	SER
1	A	159	LYS
1	A	162	SER
1	A	173	ASN
1	A	175	GLU
1	A	180	CYS
1	A	183	SER
1	A	194	ASP
1	A	197	LEU
1	A	198	CYS
1	A	220	LYS
1	A	228	LEU
1	A	246	ASN
1	A	249	ASN
1	A	251	LYS
1	A	252	ASN
1	A	262	LYS

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Mol	Chain	Res	Type
1	A	267	VAL
1	A	275	LYS
1	A	278	LYS
1	A	287	ASN
1	A	311	ASN
1	A	319	LYS
1	A	322	ASN
1	A	323	THR
1	A	335	ILE
1	A	337	GLU
1	A	339	ARG
2	B	22	THR
2	B	37	LEU
2	B	39	LEU
2	B	44	SER
2	B	50	SER
2	B	84	LYS
2	B	106	ARG
2	B	118	HIS
2	B	120	VAL
2	B	123	CYS
2	B	124	ASP
2	B	145	SER
2	B	149	LYS
2	B	152	SER
2	B	170	LEU
2	B	185	SER
2	B	211	SER
2	B	214	VAL
3	C	25	THR
3	C	38	VAL
3	C	43	SER
3	C	48	SER
3	C	63	VAL
3	C	81	SER
3	C	101	GLU
3	C	110	ASP
3	C	111	ASN
3	C	140	ASP
3	C	141	GLU
3	C	143	LEU
3	C	167	LYS

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Mol	Chain	Res	Type
3	C	180	SER
3	C	188	ASP
3	C	192	SER
3	C	194	SER
3	C	197	LEU
3	C	201	LYS
3	C	229	ARG
4	D	30	LEU
4	D	40	VAL
4	D	41	CYS
4	D	54	GLN
4	D	57	ARG
4	D	70	ILE
4	D	84	LYS
4	D	88	THR
4	D	89	ILE
4	D	91	ARG
4	D	99	ARG
4	D	100	LEU
4	D	120	ARG
4	D	121	SER
4	D	124	CYS
4	D	125	ILE
4	D	130	ASP
4	D	173	VAL
4	D	209	LEU
4	D	213	VAL
4	D	226	ILE
4	D	241	LYS
4	D	243	GLU
5	E	24	LEU
5	E	30	VAL
5	E	36	GLU
5	E	41	THR
5	E	43	SER
5	E	64	VAL
5	E	65	ILE
5	E	78	ARG
5	E	84	PHE
5	E	121	LEU
5	E	125	ARG
5	E	151	CYS

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Mol	Chain	Res	Type
5	E	154	ASN
5	E	192	LEU
5	E	198	LEU
5	E	225	SER
6	F	30	LEU
6	F	37	LEU
6	F	39	LEU
6	F	98	VAL
6	F	101	GLN
6	F	108	GLU
6	F	137	HIS
6	F	139	THR
6	F	170	LEU
6	F	182	VAL
6	F	201	VAL
6	F	214	VAL
6	F	224	GLN
6	F	243	VAL
7	G	30	VAL
7	G	39	LYS
7	G	70	LYS
7	G	98	GLU
7	G	121	LEU
7	G	122	THR
7	G	148	SER
7	G	151	CYS
7	G	154	ASN
7	G	192	LEU
7	G	196	LEU
7	G	208	VAL
7	G	225	SER
1	H	38	GLU
1	H	39	LEU
1	H	50	ARG
1	H	57	LYS
1	H	58	ARG
1	H	59	GLU
1	H	68	LEU
1	H	91	ASN
1	H	99	LEU
1	H	100	THR
1	H	109	VAL

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Mol	Chain	Res	Type
1	H	112	GLU
1	H	117	LEU
1	H	121	ASP
1	H	128	LYS
1	H	130	ASP
1	H	131	MET
1	H	139	ASN
1	H	155	ILE
1	H	157	LYS
1	H	159	LYS
1	H	166	SER
1	H	174	ARG
1	H	180	CYS
1	H	182	VAL
1	H	183	SER
1	H	198	CYS
1	H	229	ARG
1	H	234	LYS
1	H	245	ASP
1	H	249	ASN
1	H	252	ASN
1	H	254	ASN
1	H	263	ASP
1	H	274	LEU
1	H	275	LYS
1	H	276	ASP
1	H	278	LYS
1	H	309	ASN
1	H	313	ILE
1	H	314	LEU
1	H	315	ILE
1	H	320	TYR
1	H	322	ASN
1	H	335	ILE
1	H	337	GLU
1	H	345	SER
2	I	26	SER
2	I	37	LEU
2	I	40	VAL
2	I	53	THR
2	I	97	THR
2	I	106	ARG

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Mol	Chain	Res	Type
2	I	118	HIS
2	I	120	VAL
2	I	123	CYS
2	I	124	ASP
2	I	131	CYS
2	I	149	LYS
2	I	167	THR
2	I	193	SER
3	J	25	THR
3	J	38	VAL
3	J	43	SER
3	J	63	VAL
3	J	81	SER
3	J	96	VAL
3	J	101	GLU
3	J	110	ASP
3	J	111	ASN
3	J	140	ASP
3	J	141	GLU
3	J	143	LEU
3	J	180	SER
3	J	188	ASP
3	J	192	SER
3	J	201	LYS
4	K	24	ASP
4	K	30	LEU
4	K	40	VAL
4	K	42	LYS
4	K	54	GLN
4	K	57	ARG
4	K	84	LYS
4	K	88	THR
4	K	89	ILE
4	K	99	ARG
4	K	100	LEU
4	K	129	ASP
4	K	140	VAL
4	K	148	LYS
4	K	173	VAL
4	K	209	LEU
4	K	213	VAL
4	K	226	ILE

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Mol	Chain	Res	Type
4	K	241	LYS
4	K	242	VAL
4	K	243	GLU
5	L	36	GLU
5	L	41	THR
5	L	43	SER
5	L	67	GLU
5	L	70	LYS
5	L	77	SER
5	L	78	ARG
5	L	80	SER
5	L	83	LYS
5	L	84	PHE
5	L	87	THR
5	L	95	VAL
5	L	98	ASP
5	L	109	ASP
5	L	121	LEU
5	L	125	ARG
5	L	151	CYS
5	L	154	ASN
5	L	192	LEU
5	L	198	LEU
5	L	225	SER
6	M	24	ASP
6	M	41	CYS
6	M	42	LYS
6	M	95	GLN
6	M	98	VAL
6	M	101	GLN
6	M	108	GLU
6	M	137	HIS
6	M	139	THR
6	M	142	ILE
6	M	170	LEU
6	M	182	VAL
6	M	214	VAL
6	M	224	GLN
6	M	225	THR
6	M	239	VAL
6	M	243	VAL
6	M	246	LYS

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Mol	Chain	Res	Type
7	N	30	VAL
7	N	39	LYS
7	N	53	GLN
7	N	55	LYS
7	N	70	LYS
7	N	102	VAL
7	N	119	THR
7	N	121	LEU
7	N	125	ARG
7	N	154	ASN
7	N	178	GLU
7	N	182	GLU
7	N	186	LYS
7	N	192	LEU
7	N	196	LEU
7	N	208	VAL
7	N	224	LYS
1	O	37	THR
1	O	38	GLU
1	O	39	LEU
1	O	50	ARG
1	O	57	LYS
1	O	58	ARG
1	O	59	GLU
1	O	71	GLU
1	O	74	GLU
1	O	84	LYS
1	O	86	SER
1	O	91	ASN
1	O	95	LYS
1	O	100	THR
1	O	109	VAL
1	O	121	ASP
1	O	130	ASP
1	O	139	ASN
1	O	155	ILE
1	O	157	LYS
1	O	159	LYS
1	O	166	SER
1	O	170	LYS
1	O	174	ARG
1	O	180	CYS

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Mol	Chain	Res	Type
1	O	186	LYS
1	O	188	LYS
1	O	198	CYS
1	O	217	ASP
1	O	224	GLN
1	O	228	LEU
1	O	229	ARG
1	O	243	VAL
1	O	254	ASN
1	O	274	LEU
1	O	275	LYS
1	O	276	ASP
1	O	278	LYS
1	O	309	ASN
1	O	311	ASN
1	O	313	ILE
1	O	314	LEU
1	O	315	ILE
1	O	316	LYS
1	O	319	LYS
1	O	320	TYR
1	O	335	ILE
1	O	337	GLU
1	O	345	SER
2	P	26	SER
2	P	37	LEU
2	P	40	VAL
2	P	44	SER
2	P	53	THR
2	P	97	THR
2	P	118	HIS
2	P	120	VAL
2	P	148	THR
2	P	149	LYS
2	P	197	THR
2	P	209	SER
2	P	238	LYS
3	Q	25	THR
3	Q	38	VAL
3	Q	43	SER
3	Q	48	SER
3	Q	63	VAL

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Mol	Chain	Res	Type
3	Q	79	ARG
3	Q	81	SER
3	Q	101	GLU
3	Q	103	VAL
3	Q	110	ASP
3	Q	111	ASN
3	Q	122	LEU
3	Q	140	ASP
3	Q	141	GLU
3	Q	143	LEU
3	Q	165	GLN
3	Q	167	LYS
3	Q	180	SER
3	Q	188	ASP
3	Q	192	SER
3	Q	201	LYS
4	R	30	LEU
4	R	40	VAL
4	R	54	GLN
4	R	57	ARG
4	R	84	LYS
4	R	88	THR
4	R	89	ILE
4	R	99	ARG
4	R	100	LEU
4	R	120	ARG
4	R	121	SER
4	R	124	CYS
4	R	125	ILE
4	R	140	VAL
4	R	148	LYS
4	R	171	CYS
4	R	173	VAL
4	R	209	LEU
4	R	213	VAL
4	R	226	ILE
4	R	227	CYS
4	R	241	LYS
4	R	242	VAL
4	R	243	GLU
5	S	30	VAL
5	S	39	LYS

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Mol	Chain	Res	Type
5	S	55	LYS
5	S	70	LYS
5	S	78	ARG
5	S	84	PHE
5	S	122	THR
5	S	123	VAL
5	S	142	LEU
5	S	151	CYS
5	S	154	ASN
5	S	178	GLU
5	S	192	LEU
5	S	200	LYS
5	S	202	ASP
5	S	211	CYS
5	S	224	LYS
6	T	24	ASP
6	T	37	LEU
6	T	39	LEU
6	T	50	SER
6	T	84	LYS
6	T	98	VAL
6	T	101	GLN
6	T	108	GLU
6	T	139	THR
6	T	142	ILE
6	T	149	LYS
6	T	170	LEU
6	T	182	VAL
6	T	214	VAL
6	T	224	GLN
6	T	225	THR
6	T	243	VAL
7	U	30	VAL
7	U	39	LYS
7	U	70	LYS
7	U	98	GLU
7	U	112	ASN
7	U	122	THR
7	U	123	VAL
7	U	151	CYS
7	U	154	ASN
7	U	192	LEU

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Mol	Chain	Res	Type
7	U	196	LEU
7	U	200	LYS
7	U	207	LYS
7	U	208	VAL
7	U	216	GLN
1	V	39	LEU
1	V	50	ARG
1	V	57	LYS
1	V	58	ARG
1	V	59	GLU
1	V	68	LEU
1	V	69	LYS
1	V	71	GLU
1	V	72	GLU
1	V	74	GLU
1	V	84	LYS
1	V	91	ASN
1	V	95	LYS
1	V	99	LEU
1	V	100	THR
1	V	109	VAL
1	V	117	LEU
1	V	124	PHE
1	V	127	ARG
1	V	129	LYS
1	V	130	ASP
1	V	139	ASN
1	V	155	ILE
1	V	157	LYS
1	V	159	LYS
1	V	166	SER
1	V	170	LYS
1	V	174	ARG
1	V	180	CYS
1	V	185	TYR
1	V	198	CYS
1	V	210	THR
1	V	217	ASP
1	V	220	LYS
1	V	224	GLN
1	V	229	ARG
1	V	243	VAL

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Mol	Chain	Res	Type
1	V	245	ASP
1	V	247	ILE
1	V	252	ASN
1	V	254	ASN
1	V	274	LEU
1	V	275	LYS
1	V	309	ASN
1	V	313	ILE
1	V	314	LEU
1	V	315	ILE
1	V	316	LYS
1	V	320	TYR
1	V	322	ASN
1	V	335	ILE
1	V	337	GLU
1	V	345	SER
2	W	26	SER
2	W	37	LEU
2	W	40	VAL
2	W	44	SER
2	W	53	THR
2	W	97	THR
2	W	118	HIS
2	W	120	VAL
2	W	131	CYS
2	W	145	SER
2	W	149	LYS
2	W	209	SER
2	W	211	SER
2	W	239	VAL
3	X	25	THR
3	X	38	VAL
3	X	43	SER
3	X	63	VAL
3	X	81	SER
3	X	88	THR
3	X	101	GLU
3	X	108	SER
3	X	110	ASP
3	X	111	ASN
3	X	140	ASP
3	X	141	GLU

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Mol	Chain	Res	Type
3	X	143	LEU
3	X	151	VAL
3	X	165	GLN
3	X	167	LYS
3	X	180	SER
3	X	181	VAL
3	X	185	ASP
3	X	188	ASP
3	X	189	SER
3	X	192	SER
3	X	201	LYS
3	X	229	ARG
4	Y	30	LEU
4	Y	40	VAL
4	Y	41	CYS
4	Y	54	GLN
4	Y	57	ARG
4	Y	62	LYS
4	Y	70	ILE
4	Y	84	LYS
4	Y	88	THR
4	Y	89	ILE
4	Y	99	ARG
4	Y	100	LEU
4	Y	117	LYS
4	Y	120	ARG
4	Y	121	SER
4	Y	124	CYS
4	Y	125	ILE
4	Y	130	ASP
4	Y	140	VAL
4	Y	148	LYS
4	Y	209	LEU
4	Y	213	VAL
4	Y	226	ILE
4	Y	241	LYS
4	Y	242	VAL
4	Y	243	GLU
5	Z	30	VAL
5	Z	39	LYS
5	Z	55	LYS
5	Z	65	ILE

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Mol	Chain	Res	Type
5	Z	69	ASN
5	Z	70	LYS
5	Z	84	PHE
5	Z	108	ARG
5	Z	109	ASP
5	Z	111	ASN
5	Z	124	LEU
5	Z	125	ARG
5	Z	151	CYS
5	Z	154	ASN
5	Z	186	LYS
5	Z	192	LEU
5	Z	198	LEU
5	Z	225	SER
6	a	78	LEU
6	a	80	THR
6	a	84	LYS
6	a	86	ARG
6	a	88	THR
6	a	98	VAL
6	a	101	GLN
6	a	106	ARG
6	a	110	THR
6	a	120	ASP
6	a	137	HIS
6	a	145	SER
6	a	147	SER
6	a	149	LYS
6	a	170	LEU
6	a	182	VAL
6	a	214	VAL
7	b	30	VAL
7	b	31	SER
7	b	37	THR
7	b	38	VAL
7	b	39	LYS
7	b	56	SER
7	b	62	VAL
7	b	70	LYS
7	b	87	THR
7	b	96	GLN
7	b	112	ASN

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Mol	Chain	Res	Type
7	b	119	THR
7	b	121	LEU
7	b	122	THR
7	b	123	VAL
7	b	124	LEU
7	b	125	ARG
7	b	140	GLU
7	b	150	VAL
7	b	155	ASN
7	b	162	LYS
7	b	164	GLN
7	b	166	LYS
7	b	168	ASP
7	b	171	LEU
7	b	181	THR
7	b	185	SER
7	b	186	LYS
7	b	187	ASP
7	b	192	LEU
7	b	196	LEU
7	b	208	VAL
7	b	225	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	62	ASN
1	A	76	HIS
1	A	104	HIS
1	A	126	ASN
1	A	139	ASN
1	A	145	ASN
1	A	202	HIS
1	A	224	GLN
1	A	246	ASN
1	A	260	HIS
1	A	287	ASN
1	A	298	ASN
1	A	311	ASN
1	A	322	ASN
1	A	348	GLN

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Mol	Chain	Res	Type
2	B	196	HIS
2	B	232	HIS
3	C	142	GLN
3	C	155	ASN
3	C	156	ASN
3	C	228	ASN
5	E	68	ASN
5	E	141	GLN
6	F	31	GLN
6	F	103	ASN
1	H	45	ASN
1	H	126	ASN
1	H	139	ASN
1	H	146	ASN
1	H	202	HIS
1	H	235	ASN
1	H	249	ASN
1	H	254	ASN
1	H	309	ASN
1	H	348	GLN
1	H	360	ASN
2	I	78	ASN
2	I	101	GLN
2	I	121	ASN
2	I	196	HIS
2	I	231	ASN
2	I	232	HIS
2	I	236	ASN
3	J	97	GLN
3	J	155	ASN
3	J	178	GLN
5	L	33	ASN
5	L	112	ASN
5	L	141	GLN
6	M	203	GLN
7	N	216	GLN
1	O	104	HIS
1	O	126	ASN
1	O	139	ASN
1	O	145	ASN
1	O	146	ASN
1	O	202	HIS

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Mol	Chain	Res	Type
1	O	254	ASN
1	O	309	ASN
1	O	348	GLN
1	O	360	ASN
2	P	78	ASN
2	P	101	GLN
2	P	121	ASN
2	P	137	HIS
2	P	231	ASN
2	P	232	HIS
3	Q	156	ASN
3	Q	228	ASN
4	R	58	GLN
5	S	53	GLN
5	S	54	GLN
6	T	93	ASN
6	T	103	ASN
6	T	104	ASN
6	T	203	GLN
6	T	224	GLN
1	V	32	HIS
1	V	139	ASN
1	V	146	ASN
1	V	202	HIS
1	V	254	ASN
1	V	309	ASN
1	V	348	GLN
1	V	354	HIS
1	V	360	ASN
2	W	78	ASN
2	W	101	GLN
2	W	187	ASN
2	W	231	ASN
2	W	232	HIS
3	X	70	GLN
3	X	142	GLN
3	X	165	GLN
3	X	228	ASN
5	Z	53	GLN
5	Z	69	ASN
5	Z	141	GLN
6	a	58	GLN

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Mol	Chain	Res	Type
6	a	124	HIS
7	b	33	ASN
7	b	54	GLN
7	b	68	ASN
7	b	112	ASN
7	b	141	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	328/343 (95%)	0.45	15 (4%)	37 25	76, 140, 180, 206	0
1	H	321/343 (93%)	0.27	19 (5%)	28 19	122, 149, 182, 203	0
1	O	327/343 (95%)	0.16	6 (1%)	67 48	125, 151, 182, 196	0
1	V	325/343 (94%)	0.25	14 (4%)	40 26	139, 169, 200, 214	0
2	B	221/230 (96%)	0.13	10 (4%)	38 25	123, 147, 178, 193	0
2	I	202/230 (87%)	0.26	11 (5%)	31 21	119, 146, 248, 251	0
2	P	159/230 (69%)	0.39	9 (5%)	29 20	141, 168, 274, 277	0
2	W	218/230 (94%)	0.13	9 (4%)	41 27	142, 168, 219, 229	0
3	C	207/210 (98%)	0.14	7 (3%)	48 32	118, 151, 189, 201	0
3	J	192/210 (91%)	0.22	9 (4%)	36 24	123, 151, 258, 268	0
3	Q	129/210 (61%)	0.15	6 (4%)	36 24	134, 162, 271, 278	0
3	X	206/210 (98%)	0.26	11 (5%)	32 21	140, 190, 222, 233	0
4	D	136/230 (59%)	0.44	11 (8%)	18 14	81, 190, 243, 257	1 (0%)
4	K	125/230 (54%)	0.24	6 (4%)	35 24	73, 189, 212, 216	1 (0%)
4	R	126/230 (54%)	0.22	5 (3%)	42 28	72, 203, 227, 233	1 (0%)
4	Y	136/230 (59%)	0.08	6 (4%)	39 25	86, 207, 264, 283	1 (0%)
5	E	104/209 (49%)	0.30	10 (9%)	13 11	142, 184, 197, 211	2 (1%)
5	L	103/209 (49%)	0.26	5 (4%)	35 23	115, 188, 206, 218	2 (1%)
5	S	98/209 (46%)	0.13	5 (5%)	33 22	123, 205, 218, 267	2 (2%)
5	Z	103/209 (49%)	0.51	9 (8%)	16 12	146, 211, 227, 238	2 (1%)
6	F	129/321 (40%)	0.27	4 (3%)	51 34	143, 181, 202, 205	0
6	M	155/321 (48%)	0.30	10 (6%)	25 17	133, 153, 203, 252	0
6	T	146/321 (45%)	0.04	4 (2%)	56 38	170, 194, 241, 251	0
6	a	128/321 (39%)	-0.02	1 (0%)	82 68	181, 203, 209, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
7	G	101/209 (48%)	0.43	10 (9%)	13	10	146, 162, 178, 184	0
7	N	206/209 (98%)	0.29	13 (6%)	26	18	149, 183, 211, 219	0
7	U	160/209 (76%)	0.38	12 (7%)	20	15	168, 194, 251, 256	0
7	b	139/209 (66%)	0.30	11 (7%)	18	14	180, 193, 236, 242	0
All	All	4930/7008 (70%)	0.25	248 (5%)	34	23	72, 171, 227, 283	12 (0%)

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Y	126	THR	7.2
4	K	130	ASP	6.8
5	E	142	LEU	6.0
5	Z	142	LEU	6.0
3	Q	63	VAL	5.9
7	U	103	TYR	5.8
6	T	65	GLU	5.8
5	L	142	LEU	5.5
2	I	170	LEU	5.0
7	b	149	VAL	5.0
1	V	261	GLU	4.9
1	H	239	PHE	4.9
7	U	104	TYR	4.8
7	N	210	ALA	4.6
5	S	142	LEU	4.6
4	D	126	THR	4.5
1	H	283	VAL	4.5
4	D	55	TRP	4.4
5	L	44	GLY	4.4
7	G	112	ASN	4.4
3	X	133	VAL	4.3
5	E	110	THR	4.3
3	X	153	LEU	4.2
7	G	113	VAL	4.1
5	E	141	GLN	4.1
4	R	242	VAL	4.1
6	T	64	LEU	4.0
5	Z	92	ILE	4.0
6	F	132	ILE	4.0
4	R	141	ILE	3.9
4	K	242	VAL	3.9
7	N	220	SER	3.9

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Mol	Chain	Res	Type	RSRZ
5	E	111	ASN	3.8
1	H	340	ALA	3.8
5	E	112	ASN	3.8
7	U	135	PHE	3.8
1	H	237	LEU	3.7
5	E	113	GLY	3.7
6	M	116	THR	3.7
1	A	324	ALA	3.7
2	I	87	ALA	3.7
6	M	114	PHE	3.7
7	N	172	GLN	3.6
2	B	90	SER	3.6
4	R	74	GLY	3.6
7	b	88	GLY	3.5
1	H	49	ILE	3.5
4	D	154	PRO	3.5
2	B	113	TYR	3.5
7	b	156	PHE	3.5
3	X	111	ASN	3.5
7	N	208	VAL	3.4
7	G	68	ASN	3.4
1	A	49	ILE	3.4
2	W	168	ALA	3.4
4	Y	84	LYS	3.3
5	Z	48	ASP	3.3
6	M	74	GLY	3.3
7	b	150	VAL	3.3
2	W	167	THR	3.3
3	Q	64	THR	3.3
7	G	115	PHE	3.3
3	J	183	GLU	3.3
2	W	215	THR	3.3
7	N	166	LYS	3.3
1	V	187	PHE	3.2
1	A	177	PHE	3.2
5	L	109	ASP	3.2
3	C	137	PRO	3.2
1	A	142	LYS	3.1
7	b	44	GLY	3.1
1	H	292	VAL	3.1
1	V	333	VAL	3.1
5	Z	38	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
7	G	110	SER	3.1
3	X	82	GLY	3.1
1	O	228	LEU	3.1
5	Z	141	GLN	3.1
6	a	76	PHE	3.1
3	Q	204	TYR	3.1
2	B	87	ALA	3.0
7	N	222	VAL	3.0
2	W	214	VAL	3.0
5	S	30	VAL	3.0
2	I	210	LEU	3.0
7	U	188	SER	3.0
4	D	122	ASP	3.0
3	X	62	PRO	2.9
2	I	198	PHE	2.9
7	b	46	THR	2.9
3	J	208	LYS	2.9
1	V	328	TYR	2.9
5	S	126	THR	2.9
3	J	214	VAL	2.9
2	B	191	LEU	2.9
3	J	65	LEU	2.9
7	b	123	VAL	2.9
4	D	114	TYR	2.9
3	X	160	ARG	2.9
7	b	86	SER	2.9
1	A	334	LYS	2.9
3	X	154	LEU	2.9
1	O	31	ARG	2.9
1	O	188	LYS	2.9
4	Y	125	ILE	2.9
1	A	93	LEU	2.8
4	R	142	VAL	2.8
1	H	95	LYS	2.8
1	H	68	LEU	2.8
4	D	130	ASP	2.8
1	O	167	LEU	2.8
1	A	101	GLY	2.7
4	D	115	CYS	2.7
2	I	243	VAL	2.7
2	P	234	PRO	2.7
3	C	62	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	P	26	SER	2.7
7	U	82	SER	2.7
7	b	154	ASN	2.7
6	M	134	ALA	2.7
1	O	353	ILE	2.7
4	K	126	THR	2.7
6	F	116	THR	2.7
7	G	85	GLY	2.7
1	V	298	ASN	2.7
6	M	115	CYS	2.7
1	A	274	LEU	2.7
5	S	111	ASN	2.7
2	I	115	CYS	2.7
1	V	299	ASN	2.7
3	J	74	SER	2.6
1	H	235	ASN	2.6
2	P	229	ASN	2.6
5	Z	111	ASN	2.6
2	P	27	GLY	2.6
7	U	140	GLU	2.6
3	J	23	ALA	2.6
4	D	242	VAL	2.6
7	b	45	SER	2.6
5	L	141	GLN	2.6
3	J	136	PHE	2.6
2	I	55	GLN	2.6
4	Y	127	GLY	2.6
5	E	108	ARG	2.6
4	K	89	ILE	2.5
6	T	125	TYR	2.5
5	S	141	GLN	2.5
1	H	324	ALA	2.5
6	M	158	PRO	2.5
7	G	111	ARG	2.5
7	U	211	CYS	2.5
4	Y	139	GLU	2.5
4	K	131	ILE	2.5
7	U	53	GLN	2.5
1	O	312	SER	2.5
1	H	232	ILE	2.5
2	I	226	TYR	2.5
2	W	213	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
4	R	75	SER	2.4
2	W	135	TRP	2.4
6	F	135	TRP	2.4
3	J	137	PRO	2.4
1	A	318	GLU	2.4
1	H	284	SER	2.4
7	U	193	SER	2.4
7	N	152	LEU	2.4
1	V	267	VAL	2.4
7	N	67	TYR	2.4
3	Q	23	ALA	2.4
7	G	67	TYR	2.4
7	b	97	ALA	2.4
1	H	120	GLU	2.4
1	V	148	GLU	2.4
2	P	231	ASN	2.4
7	N	153	LEU	2.4
5	Z	126	THR	2.3
2	I	196	HIS	2.3
5	E	48	ASP	2.3
3	C	168	VAL	2.3
6	F	20	ALA	2.3
4	Y	114	TYR	2.3
1	V	281	GLN	2.3
2	W	84	LYS	2.3
7	N	113	VAL	2.3
7	N	167	VAL	2.3
5	E	85	GLY	2.3
1	A	231	TYR	2.3
3	X	80	PHE	2.3
2	W	169	ALA	2.3
7	G	82	SER	2.3
2	P	226	TYR	2.3
1	V	175	GLU	2.2
7	N	219	SER	2.2
1	V	31	ARG	2.2
3	J	75	ASP	2.2
7	U	115	PHE	2.2
3	X	132	SER	2.2
1	H	169	LEU	2.2
7	U	25	THR	2.2
1	A	284	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	148	GLU	2.2
1	H	249	ASN	2.2
1	V	248	ASN	2.2
7	U	68	ASN	2.2
2	B	165	GLY	2.2
1	H	316	LYS	2.2
3	Q	110	ASP	2.2
5	Z	93	THR	2.2
7	N	223	THR	2.2
2	B	159	SER	2.2
3	C	97	GLN	2.2
6	M	218	SER	2.2
6	M	23	LEU	2.2
1	A	91	ASN	2.2
3	C	187	LYS	2.2
5	Z	97	ALA	2.2
4	D	41	CYS	2.2
6	T	133	ASP	2.2
3	Q	206	LYS	2.1
1	A	126	ASN	2.1
5	E	84	PHE	2.1
4	D	56	VAL	2.1
7	G	121	LEU	2.1
1	V	107	ALA	2.1
2	B	186	TRP	2.1
2	B	112	THR	2.1
2	W	170	LEU	2.1
3	C	59	GLY	2.1
6	M	54	GLY	2.1
2	I	47	PHE	2.1
2	P	214	VAL	2.1
4	K	123	TYR	2.1
3	C	171	ALA	2.1
3	X	162	ALA	2.1
6	M	69	GLY	2.1
2	I	234	PRO	2.1
1	A	233	SER	2.1
2	B	102	LEU	2.1
5	L	49	TYR	2.1
2	P	178	PHE	2.1
1	H	338	ASN	2.0
1	V	225	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	232	ILE	2.0
1	H	305	ILE	2.0
3	X	52	TRP	2.0
2	B	157	ALA	2.0
4	D	150	PRO	2.0
2	P	21	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CA	F	401	1/1	-	-	190,190,190,190	1
8	CA	F	402	1/1	-	-	112,112,112,112	1
8	CA	H	401	1/1	-	-	185,185,185,185	1
8	CA	M	401	1/1	-	-	136,136,136,136	1
8	CA	T	401	1/1	-	-	233,233,233,233	1
8	CA	T	402	1/1	-	-	235,235,235,235	1
8	CA	a	401	1/1	-	-	241,241,241,241	1
8	CA	a	402	1/1	-	-	178,178,178,178	1

6.5 Other polymers [i](#)

There are no such residues in this entry.